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Simulation of Infrared Spectra

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Programs have been developed to simulate absorption and emission spectra of atmospheric and combustion product species. The programs use tabulated constants of the molecules of interest to calculate transition frequencies and line strengths as a function of temperature. Asymmetric rotors and linear molecules have been included. The calculated emission and absorption spectra can be compared to experimental spectra and can be used to predict spectral shifts due to isotopic substitution. Results for a variety of materials and conditions are presented.

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SIMULATION OF INFRARED SPECTRA

INTRODUCTION

The Naval Research Laboratory supports a number of programs concerning the infrared (IR) spectral characteristics of the materials produced by the combustion of a variety of types of fuels. These programs include measurements of the IR absorption and emission spectra of the combustion plumes of various materials under differing conditions. In an effort to more fully understand the combustion processes, a spectral simulation effort has been initiated. The purpose of this effort is to develop the capability of simulating IR spectra for comparison with experimental results. The molecules of interest in the simulation effort are atmospheric constituents and their isotopic variants. Programs have been developed to simulate the absorption and emission spectra of these materials at different temperatures and under varying conditions. This report discusses the structure of the programs and the input data which are required. Results of calculations for a variety of materials and conditions are also presented.

PROGRAM STRUCTURE

Programs have been developed to calculate the spectra of isotopic variants of water (H_2O, HDO, and D_2O), CO_2, and $HC\ell$ and $DC\ell$. All programs are written in FORTRAN and run on the IBM AT computer. In the sections below, the theoretical underpinning of each set of programs is discussed. A general discussion of the program structure follows and then the details of program implementation are outlined. Copies of the program codes are included in the Appendix. Also in the Appendix are sample parameter files showing the structure and formatting of the input files. For both water and CO_2, actual input and output files are included. The discussion for each molecule assumes that an absorption spectrum is to be calculated. The changes in the program necessary to calculate an emission spectrum are detailed.

Calculations For Isotopic H_2O

The most difficult calculation is that for water which is an asymmetric rotor. King, Hainer and Cross originally determined expressions for the energy levels of an asymmetric rotor [1]. Each energy level is characterized by J, the total angular

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momentum, and by two pseudo-quantum numbers, K_{-1} and K_1. The pseudo-quantum numbers are used to distinguish between the $2J+1$ levels that have the same value of J. A level is labelled by the values of K to which it corresponds in the prolate symmetric rotor (K_{-1}) and in the oblate symmetric rotor (K_1). These two values are combined to define an asymmetry parameter τ

$$\tau = K_{-1} - K_1$$

The parameter τ assumes the values $-J$, $-J+1$, ..., 0, ..., $J-1$, J. The energy levels are ranked in order by the value of τ with the lowest energy level for a given J being that with $\tau = -J$ and the highest that with $\tau = J$. In addition, τ serves as an index to the parity of the levels. For molecules belonging to the C_{3v} point group, those levels with even $|\tau|$ are symmetric with respect to interchange of identical nuclei and those with odd $|\tau|$ are antisymmetric with respect to interchange of identical nuclei.

Cross, Hainer, and King also derived a means of calculating line strengths for the lines in an asymmetric rotor spectrum [2]. The line strength calculation requires the evaluation of the matrix elements of the direction cosines which are the elements of an orthogonal transformation from molecule-fixed to space-fixed coordinates. Application of their method allows calculation of the line strength of a particular transition as a function of the asymmetry of the rotor.

The starting point for the programs described herein was a program coded by Y. Endo and kindly provided by J.E. Butler (Code 6170, Chemistry Division, Naval Research Laboratory, Washington, D.C.). The program was designed for analysis of microwave spectra of asymmetric rotors. The calculation of the transition frequencies was not altered, but the intensity calculation required considerable modification (e.g., in the original program the temperature could not be varied). The dependence of the line intensity S for an absorption at the frequency ν is given by the following expression (note that, since only relative intensities from the calculation are used, proportionalities

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may be used instead of equalities):

$$S \propto (\frac{\nu}{\nu_o})[1-\exp(-c_2\nu/T_o)] \, g''F \, Q_R(T_o)\exp(-c_2E_R''/T_o)\ell^2 \, S_v^0(T_o) \qquad (1)$$

ν_o = band center

c_2 = second radiation constant

    = 1.438786 cm K

T_o = reference temperature = 296K

 g'' = statistical weight of lower state

 F = vibration - rotation interaction constant

$Q_R(T_o)$ = rotational partition function at T_o .

E_R'' = rotational energy of lower state

ℓ^2 = direction cosines matrix element connecting lower and upper states

$S_v^0(T_o)$ = band strength at T_o

The band strength depends on the following factors:

$$S_v^0 \propto \frac{\nu_0 \, |R|^2}{Q_v(T_o)} \exp(-c_2G_v''/T_o) \qquad (2)$$

R = matrix element of the rotationless electric dipole moment

G_v'' = vibrational energy of lower state

$Q_v(T_o)$ = vibrational partition function at T_o

Some comment is necessary on several of the terms included above. The term in square

brackets in equation (1) is the induced emission term. It is negligibly small for the case

in which $c_3\nu >> T$ but is included for completeness. The statistical weight or nuclear

statistics factor g'' depends on the symmetry of the lower state and will be discussed

further below. The vibration-rotation interaction factor will be assumed to be equal to

one in most cases. The band strength for the vibrational transition is available from

tabulated values.

The temperature dependence of the line strength arises through the rotational and

vibrational Boltzmann factors and the rotational and vibrational partition functions, as

well as a small effect from the induced emission term. Excluding the induced emission

term. McClatchey [3] gives the temperature dependence as

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$$S(T) = \frac{S(T_o)\, Q_v(T_o)Q_R(T_o)}{Q_v(T)\, Q_R(T)} \exp\left[\frac{c_2 E''\,(T-T_o)}{T\, T_o}\right] \qquad (3)$$

where E'' is the lower state energy, including both vibrational and rotational energy. This dependence differs by a factor of T_o/T from that given in some sources ([4], for example) because the units to be used for S_v^0 are cm/molecule rather than $cm^{-2}\ atm^{-1}$. The temperature dependence for the bands in the water molecule can be written in somewhat simpler terms for two reasons: (1) the partition functions at T_o are constants and can be omitted since only relative strengths are being calculated; and (2) the vibrational Boltzmann factor is equal to one because all bands considered have the vibrational ground state as the lower state. Note that the temperature dependence of the induced emission term can be accounted for by multiplying by the ratio of that term at temperature T to that at temperature T_o, cancelling out the T_o term. The resulting expression for the line intensity at a temperature T is

$$S \propto \frac{\nu}{\nu_0}\, [1-\exp(-c_2\nu/T)]\ \frac{g''\ell^2}{Q_R(T)Q_v(T)}\, \exp(-c_2 E_R''/T)\, S_v^0(T_o) \qquad (4)$$

The program which calculates spectra for isotopic water reads input data from a parameter file. This file identifies the molecule for which the spectrum is to be calculated and supplies the information necessary for the simulation; for a complete description of the parameter file, see below. The program calculates the transition frequencies and the line intensities. All lines with frequencies within the specified range and intensities greater than the chosen minimum are stored. After all lines have been calculated, the stored lines are sorted in order of increasing frequency. The lines are then grouped into bins of equal width with the summed intensity of all lines within the bin at the center of the bin. A Gaussian lineshape is applied to the intensity to adjust the resolution for comparison with experimental spectra. An output file is then written for plotting the spectrum.

The parameter file contains the necessary inputs for the calculation. The parameters are discussed here in the order in which they appear in the parameter file.

See pages A2 and A3 for sample parameter and input files. ISOTOPE identifies the particular isotope under consideration: 161 for H_2O, 262 for D_2O, and 162 for HDO. The upper and lower state rotational constants and centrifugal distortion constants are read into the array PAR (I). NBINS is the number of bins of equal width into which the frequency range is divided. WIDTH is the halfwidth of the Gaussian lineshape which is applied. The variable IITY codes the band type of the vibrational transition - 100 for type A transitions, 010 for type B transitions, and 001 for type C transitions. The minimum and maximum values of J are JMIN and JMAX. The maximum change allowed in τ is KTAU. The allowed frequency range is determined by the minimum and maximum frequency values FMIN and FMAX. The band center of the vibrational transition is FNUZ. STMIN is the minimum strength requirement for transitions to be stored. The temperature for the simulation is TT and the band strength for the transition is BS. The fundamental vibrational frequencies of the molecule are FNU1, FNU2, and FNU3. After the data have all been read in, they are printed to the screen so that it may be verified that the values are correct.

The program calculates frequencies and intensities for each branch in turn with the R branch first, followed by the P branch and then the Q branch. Once calculated, the frequency is tested to determine whether it falls between the limits of the frequency range. If so, a level name is determined and the strength is calculated. The strength calculation is divided into a number of steps. The direction cosines matrix element is calculated and multiplied by the rotational Boltzmann factor divided by the rotational partition function. The energy used in the Boltzmann factor is the initial state rotational energy ELI. The result of this calculation is multiplied by the nuclear statistics factor to give the parameter STRENGTH. The value of the statistical weight factor is determined by symmetry of the levels under interchange of identical nuclei and is indexed by the oddness or evenness of $|\tau|$. Table 1 gives the statistical weight factors for the isotopes of water. As STRENGTH for each level is determined, the values are summed to give TOTINT. To compare intensities correctly for different isotopes, the

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intensities must be normalized by TOTINT. This is accomplished by dividing the strength

of each line by TOTINT in the SORT subroutine. The calculation of the line intensity is

completed by multiplying STRENGTH by the frequency, the induced emission term and the

band strength, then dividing by the frequency of the band center and the vibrational

partition function. Note that dividing by the band center is required because the band

center is included in the tabulated $S_v^0(T_o)$ value.

After the line intensity is calculated, that value is compared to STMIN; if it

exceeds the minimum strength criterion, the frequency, strength, and level name are

stored. This process is continued until all lines in all three branches have been

calculated. The line counter NLINE is incremented each time a line is stored. After all

lines have been calculated, the lines are arranged in order of increasing frequency by the

SORT subroutine. The SORT subroutine also performs the normalization by TOTINT

described above. Because this normalization occurs after the comparison of the

calculated line intensity to STMIN, the minimum strength value in the lines listed in the

program output may not correspond directly to STMIN. The PRINT subroutine then

prints out information for each stored line: the band type; the branch; the final and

initial values of J, K_{-1}, and K_1; the transition frequency; the calculated strength; and the

relative strength calculated by dividing each line strength by the maximum line strength.

Next the subroutine BINSORT sorts all lines into bins of equal width, that width being

(FMAX-FMIN)/NBINS. The SHAPE subroutine applies a Gaussian lineshape of halfwidth

WIDTH to the summed intensity at the center of each bin. The total intensity of each

bin is calculated as SMOOTH(I) after application of the lineshape. The SHAPE subroutine

also writes an output file containing FMIN, FMAX, NBINS, and SMOOTH(I), I=1 to

NBINS.

The program described above must be modified to calculate an emission spectrum

rather than an absorption spectrum. There is of course no change in the transition

frequencies. The population of the emitting species is that of the upper state rather

than the lower state. The energy used in the rotational Boltzmann factor is now the

final state rotational energy ELF rather than ELI (the terminology of the absorption process is retained; "final state" actually refers to the upper state). Since the molecule must also be in the excited vibrational state to emit, a vibrational Boltzmann factor $\exp(-c_2*FNUZ/TT)$ must be used. The induced emission term is not used for the emission calculation. The index for the statistical weight factor is applied to the upper state rather than the lower state. In emission, a factor of ν^4 rather than ν is used in the intensity calculation [5]. With the exception of these modifications, the program for emission is the same as that for absorption.

Calculations For CO_2

The calculation for a linear molecule is considerably simpler than that for an asymmetric rotor since expressions for the energy and the intensity can be expressed in closed form. The expression for the energy [6] is

$$E(J) = BJ(J+1) - DJ^2(J+1)^2 + HJ^3(J+1)^3 \qquad (5)$$

Values of the constants are given in the literature. For Σ states, the calculation is straightforward. In calculating energies for Π states, the effect of ℓ-type doubling must be considered [6]. Separate constants are tabulated for e and f sublevels of Π states so both manifolds may be calculated.

In analyzing a particular transition, attention must be paid both to which levels are populated and to the selection rules governing the transition. Σ_u^+-Σ_g^+ transitions are straightforward because the ℓ-type doubling is absent; only P and R branches appear. For Π_u-Σ_g^+ transitions, a Q-branch appears in addition to the P and R branches. For molecules such as CO_2 with the spins of the nuclei equal to zero, only the symmetric levels with respect to interchange of equivalent nuclei are occupied. The selection rules require the combination of symmetric with symmetric levels. The occupied levels in the Σ state are those with even J and the absorptions terminate in the e sublevels of the upper state levels with odd J for the P and R branches. The Q branch transitions terminate in the (symmetric) f sublevels of the upper state levels with even J. For a Π_g-Π_u transition, P, Q, and R branches are allowed. The symmetric levels for a Π state

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are e sublevels with odd J, f sublevels with even J. Thus two sets of P and R branches arise - an e-e set with odd J in the lower state and an f-f set with even J in the lower state. Since the Q branch transitions must connect two symmetric levels, the e <-> f selection rule is followed. The Q transitions with odd J originate in e sublevels and terminate in f sublevels. The Q transitions with even J originate in f sublevels and terminate in e sublevels.

The expression for the intensity calculation for CO_2 bands is given explicitly by Rothman [7].

$$S = \frac{\nu}{\nu_o} S_v^0 \, S_{J\ell} \exp(-c_2 \, E_R'' T_o) \, [1-\exp(-c_2 \nu \, T_o)] \, \frac{F}{Q_R(T_o)} \tag{6}$$

$$\text{where} \quad S_v^0 = \frac{8\pi^3 \, g'' I_a}{3hc \, Q_v(T_0)} \, \nu_0 \, |R|^2 \, \exp(-c_2 G_v'' \, T_0) \tag{7}$$

All terms are as def.ned previously; $S_{J\ell}$ is the Hönl-London factor and I_a is the isotopic abundance. We will consider only the isotope containing ^{12}C and ^{16}O; the constants will be dropped since only relative values are of importance. The temperature dependence is introduced in the same manner described above for H_2O. One complication in the CO_2 case is the fact that the lower state is not the ground vibrational state in all cases. That means that the vibrational Boltzmann factor which is included in the band strength may not be equal to one. In changing temperatures, it is necessary to divide by $\exp(-c_2 G_v'' \, T_o)$ and to multiply by $\exp(-c_2 G_v'' \, T)$ to calculate correctly the population in the lower state at a temperature T.

The initial section of the program reads input data from a parameter file. The parameters are discussed here in the order in which they appear in the parameter file. See pages A40 and A41 for sample parameter and input files. The first parameter read is ID which identifies the type of band to be calculated: ID=11 for a $\Sigma_u^+-\Sigma_g^+$ band; ID=22 for a $\Pi_u-\Sigma_g^+$ band; ID=23 for a $\Pi_g-\Pi_u$ band. If ID=11, only P and R branches are calculated; if ID=22 or ID=23, P,Q, and R branches are calculated. The next set of parameters contains the upper state constants (BU', DU', and HU') to be used for the

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calculation of energy levels. For the $\Pi_u-\Sigma_g^+$ transition, the upper state energy levels are those for the e sublevel for the P and R branches. For the $\Pi_g-\Pi_u$ transition, two separate parameter files must be used for P and R branches - one using the e sublevels for odd J and one using the f sublevels for even J. The next parameters read are BUQ, DUQ, and HUQ, the upper state levels used to calculate Q branch transitions. For the $\Pi_u-\Sigma_g^+$ transition, these are for the upper state f sublevels. For each of the e-e and f-f pairs for the $\Pi_g - \Pi_u$ transition, the alternate set of sublevels is used for the Q branch upper state since the e<->f selection rule is followed. The final set of parameters BL, DL, and HL is used for the calculation of the lower state energy levels. The next set of entries in the parameter file gives minimum and maximum values of J (JMIN and JMAX) and of the frequency (FMIN and FMAX). Note that in the energy level and transition frequency calculations, J is incremented by 2. The minimum value of J thus determines whether the J values will be odd or even. The following three frequencies FNU1, FNU2, and FNU3 are the fundamental frequencies of the molecule. The next line gives the band center frequency (FNUZ) and the vibrational energies of the lower (FLOW) and upper (FHIGH) states involved in the transition. Next the band strength SV and temperature TT are input. For the $\Pi_g - \Pi_u$ transition, the band strength is equally split between the e-e and f-f pairs. The final line in the parameter file contains NBINS and WIDTH.

Following printing of the input data to the screen, three sets of energy levels are calculated for the indicated range of J: EU(I), the upper state levels; EL(I), the lower state levels; and EUQ(I), the upper state levels of the other sublevel set for calculation of the Q branch transitions. Changes in rotational energies for P and R branches (EROTP and EROTR) are calculated; for transitions involving a Π state, the changes in rotational energy for the Q branch (EROTQ) are also calculated. The vibrational Boltzmann factor and the rotational and vibrational partition functions are calculated at T_2 and at T. For the absorption calculation, the vibrational Boltzmann factor uses FLOW. In a series of loops, the frequencies and intensities of the individual lines in

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each branch are calculated. One of the factors in the strength calculation is the Hönl-London factor. The Hönl-London factor depends on both ΔJ and $\Delta \ell$. The values for the bands of CO_2 which are considered are given in Table 2 with J representing the lower state quantum number. If the frequency of the transition is within the frequency range from FMIN to FMAX, the frequency, strength, and line label are stored. The SORT, PRINT, BINSORT, and SHAPE subroutines are analogous to those described above for the water calculation.

The transformation from absorption to emission requires the same sort of changes as in the water case. The induced emission term is not used. The vibrational and rotational Boltzmann factors use upper state energy levels rather than lower state energy levels. In the intensity calculation, ν^4 replaces ν. The remainder of the calculation is identical to that for absorption.

Calculations for HCℓ and DCℓ

The calculations for the diatomics HCℓ and DCℓ are straightforward and will not be described in detail here. Only the $^{35}Cℓ$ isotope was included and only emission spectra were calculated.

Program Listings

Copies of all the programs used are included in the Appendix. The executable file ASYMABS was used for absorption calculations for the water isotopes. It was formed by linking ASYMABS + ASYMSUB + SHAPE + BINSORT. The emission calculations for water used ASYMEMS, forming by linking ASYMEMS + ASYMSUB + SHAPE + BINSORT. The corresponding absorption (emission) program for CO_2 was CO2ABS (CO2EMS), formed by linking CO2ABS (CO2EMS) + CO2SUB + CO2SHAPE + CO2BSORT. The HCℓ program linked HCLEMS + HCLSUB + HCLSHAPE + HCLBSORT.

The Appendix also includes Sample Parameter Files for H_2O and CO_2 showing the structure of the input data files and the formats used for the variables. In addition, there are actual examples of input data files H2ONU1 and CO2NU3 used for the ν_1 band of H_2O and the ν_3 band of CO_2. The sample output files generated by running

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ASYMABS and CO2ABS respectively are also shown. These may be useful as tests in trying to implement the programs.

RESULTS AND DISCUSSION

The input parameters for the three isotopes of water were collected from a variety of sources, since no one reference was identified in which a complete set for the bands under consideration was compiled. The region of the spectrum selected for consideration was 0 - 5000 cm^{-1}. The bands that make a significant contribution in this region can be identified from the AFGL band strength listing. The most recent version for the H_2O bands was the 1980 update [8]. The four bands with a band strength greater than 0.5% of the largest were used in the calculation. These are the three fundamentals and the first overtone of the bending mode. The $\nu_2+\nu_3$ combination band has significant intensity and is centered at 5331 cm^{-1}. Although the lower frequency edge extends beyond 5000 cm^{-1}, this band was not found to make a significant contribution. The pure rotational spectrum was not included.

The rotational and vibrational parameters used for the H_2O calculations are given in Table 3. For the H_2O calculations, centrifugal distortion constants are included for all bands. The corresponding parameters for D_2O are given in Table 4, but centrifugal distortion constants are not included. Note that the band strengths are from a calculation by Wilemski [14] because experimental values could not be found. The $2\nu_2$ band is omitted because no band strength could be found; by analogy to H_2O and HDO, it would make a small contribution at most. Table 5 contains the constants for HDO. Note that each band has both A and B type character; separate band strengths are given for each contribution.

The results of calculations for absorption by H_2O at 296K, 1000K, and 1730K are shown in Fig. 1. The intensity is given in arbitrary units; the intensities of the absorption spectra at different temperatures are correctly scaled relative to each other. The width parameter here is 2 cm^{-1}, corresponding to a resolution of 4 cm^{-1}. The lowest frequency band at 1594 cm^{-1} is the ν_2 bending mode. The very small

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contribution from $2\nu_2$ lies at 3155 cm^{-1}; it can be seen in 296K spectrum. The ν_1 and ν_3 bands overlie one another in the 3500-4000 cm^{-1} region. As the temperature increases, the spectra broaden as higher J levels are populated and absorb. The intensity of the absorption decreases as the temperature increases because of the decrease in population of the absorbing state. To determine the accuracy of the calculated spectra, the frequencies of lines in the calculated spectra were compared to tabulated values for each of the bands studied. The calculated values agreed with literature values to within 1 cm^{-1} in most cases with some deviations of 3-4 cm^{-1} observed. The results were not as good for individual line strengths. Variations of 50% or more were noted in comparing calculated and literature values. The purpose of this study, however, was to determine the region in which emission occurs rather than the line-by-line strength of particular portions of the spectrum. The accuracy achieved is certainly adequate for that purpose.

Emission spectra at 1730K are shown for all three isotopes in Fig. 2. The substitution of one D for H in water shifts ν_1 from 3657 cm^{-1} to 2724 cm^{-1}, giving three distinct bands. In going to D_2O, once again ν_1 and ν_3 are in the same region but all bands are shifted to lower frequency. Again all spectra are scaled correctly relative to ea h other and correspond to a resolution of 4 cm^{-1}. It is clear from Fig. 2 that changing from H_2O to D_2O shifts the most intense absorption band into a significantly different region of the spectrum. Fig. 3 shows a composite emission spectrum at 1730K for an equimolar mixture of H_2O and D_2O.

Table 6 gives the rotational and vibrational constants for CO_2. The bands included are those five for which $S_V^0 > 10^{24}$ cm/molecule. Three of these are Σ-Σ transitions with one Π-Σ transition and one Π-Π transition. The lower state for the Π-Π transition is not the ground vibrational state but instead is the 01101 state (for band notation, see [3]). Absorption spectra calculated at 296K, 1000K, and 1730K are shown in Fig. 4, correctly scaled relative to one another. The most prominent band at 2349 cm^{-1} is the ν_3 fundamental. The ν_2 fundamental appears at 667 cm^{-1} and small contributions are made

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by combination bands in the 3600-3700 cm^{-1} region. As the temperature is increased. the absorption decreases because of the smaller number of molecules in the lower vibrational state. The relative importance of the 2300 cm^{-1} peak increases relative to the 667 cm^{-1} peak because of the contribution made to the higher frequency peak by the Π-Π transition originating in the 01101 state. This excited lower state has a higher population at the higher temperature and the absorption due to this transition therefore is increased. Figure 5 shows emission due to CO_2 at 1000K and 1730K with correct relative scaling. The 2300 cm^{-1} feature is again the predominant one with its importance relative to the 667 cm^{-1} band increasing with increasing temperature. The contribution due to the 3600-3700 cm^{-1} peaks is small even at 1730K. Figure 6 shows on an expanded scale the main CO_2 band with emission calculated at 1730K and absorption calculated at 296K. The maximum value of each spectrum is individually scaled to a value of 10. If a material producing hot CO_2 were burned and the spectrum observed through an atmospheric path, the cold CO_2 in the atmosphere would absorb the radiation making up the central portion of the emission spectrum. The observed spectrum would show only the wings of the hot CO_2 spectrum, as shown in the lower panel of Fig. 6.

Table 7 gives the rotational and vibrational constants used to calculate the HCℓ and DCℓ spectra. The calculation also used a vibration-rotation interaction constant expression [22]:

$$F = 1 - 2.5599 \times 10^{-2} \, m + 3.203 \times 10^{-4} \, m^2 \tag{8}$$

Emission spectra for HCℓ and DCℓ at 1730K are shown in Fig. 7. Again it is clear that deuteration of HCℓ shifts the emission into a different region of the spectrum.

CONCLUSIONS

Spectral simulation programs have been developed which correctly calculate the spectra of species produced in the combustion of a variety of fuels. The programs calculate both positions and intensities in the vibrational-rotational spectra of isotopic forms of H_2O, CO_2, and HCℓ. The calculated values of the frequencies agree well with

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tabulated values while the agreement of intensities with literature values is not as good. As expected, the regions of emission and absorption shift markedly with isotopic substitution. The relative importance of particular transitions varies with temperature. The simulated spectra can be combined to mimic observation through an atmospheric path where both emission and absorption due to the same species are important.

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APPENDIX

The Appendix contains program listings, sample inputs, and sample outputs for the programs described in the preceding report. Contents of the Appendix are listed below.

17

SAMPLE PARAMETER FILE FOR WATER


```
ISOTOPE
PAR(1)          PAR(2)          PAR(3)
PAR(4)          PAR(5)          PAR(6)
PAR(7)          PAR(8)          PAR(9)
PAR(16)         PAR(17)         PAR(18)
PAR(19)         PAR(20)         PAR(21)
PAR(22)         PAR(23)         PAR(24)
NBINS[I5]       WIDTH[F10.6]
IITY[I4]        JM_N[I4]        JMAX[I4]            KTAU[I4]
FMIN[F10.4]     FMAX[F10.4]     FNUZ[F10.4]
STMIN[E12.3]    TT[F10.4]       BS[F10.4]
FNU1[F10.4]     FNU2[F10.4]     FNU3[F10.4]
```


```
ISOTOPE = isotope code
PAR(1),PAR(2),PAR(3) = A,B,C constants for upper state
PAR(4) - PAR(8) = distortion constants for upper state
PAR(16),PAR(17),PAR(18) = A,B,C constants for lower state
PAR(19) - PAR(23) = distortion constants for lower state
NBINS = number of bins
WIDTH = Gaussian halfwidth
IITY = band type
JMIN,JMAX = minimum and maximum values of J
KTAU = maximum change in TAU
FMIN,FMAX = minimum and maximum values of frequency
FNUZ = band center
STMIN = minimum strength
TT = temperature
BS = band strength
FNU1,FNU2,FNU3 = fundamental frequencies
```

18

SAMPLE INPUT FILE H2ONU1

```
161
27.12217            14.3047            9.1045
0.001233            -0.0053874          0.03023
0.00049987          0.0012405          0.0
27.880678           14.521689          9.277459
0.00124894          -0.0057655          0.0325199
0.00050838          0.0013007           0.0
5000   2.0
010    0   25    5
0000.        5000.        3657.053
1.50               296.        48.62
3657.053   1594.778   3755.93
```

OUTPUT FROM PROGRAM ASYMABS.FOR

PARAMETER FILE = H2ONU1

OUTPUT FILE = H2OANU1

ISOTOPE = 161

UPPER STATE CONSTANTS

A   =   27.1222   B   =   14.3047   C   =   9.1045
DLJ =   0.00123300   DLJK=   -0.00538740   DLK =   0.03023000
DSJ =   0.00049987   DSK =   0.00124050

LOWER STATE CONSTANTS

A   =   27.8807   B   =   14.5217   C   =   9.2775
DLJ =   0.00124894   DLJK=   -0.00576550   DLK =   0.03251990
DSJ =   0.00050838   DSK =   0.00130070

SELECTION RULES   F   T   F
J RANGE   0 TO   25

MAX. DELTA TAU   5
FREQ. RANGE   0.0000 TO 5000.0000 CM-1
BAND ORIGIN   3657.0530 CM-1
NU #1   3657.0530 CM-1
NU #2   1594.7780 CM-1
NU #3   3755.9300 CM-1
MIN. STRENGTH   1.500000
TEMPERATURE   296.00
NBINS   5000
WIDTH   2.000000

        0
        1
        2
        3

20

```
   4
   5
   6
   7
   8
   9
  10
  11
  12
  13
  14
  15
  16
  17
  18
  19
  20
  21
  22
  23
  24
  25
        TOTAL NUMBER OF LINES =      19

        TOTAL BAND INTENSITY = 7.5561E-01

     B    P      3  0  3      4  1  4   .   3566.55133    2.288E+00   0.6224
     B    P      2  1  2      3  0  3       3598.12016    2.048E+00   0.5572
     B    P      1  0  1      2  1  2       3600.96185    2.330E+00   0.6340
     B    Q      3  1  2      3  2  1       3615.21502    2.070E+00   0.5632
     B    Q      3  0  3      3  1  2       3618.02353    2.131E+00   0.5797
     B    Q      1  0  1      1  1  0       3638.08552    2.820E+00   0.7672
     B    Q      1  1  0      1  0  1       3674.65685    3.118E+00   0.8482
     B    Q      3  1  2      3  0  3       3690.60424    2.634E+00   0.7165
     B    Q      3  2  1      3  1  2       3691.35115    2.591E+00   0.7049
     B    R      2  1  2      1  0  1       3711.08686    3.149E+00   0.8566
     B    R      3  0  3      2  1  2       3711.89401    2.816E+00   0.7662
     B    R      4  1  4      3  0  3       3740.84666    3.676E+00   1.0000
     B    R      2  2  1      1  1  0       3746.18036    2.904E+00   0.7900
     B    R      5  0  5      4  1  4       3751.52891    3.135E+00   0.8529
     B    R      6  1  6      5  0  5       3770.55376    2.453E+00   0.6674
     B    R      4  2  3      3  1  2       3777.88815    2.037E+00   0.5541
     B    R      3  3  0      2  2  1       3800.25831    2.956E+00   0.8043
     B    R      4  3  2      3  2  1       3818.54410    2.003E+00   0.5449
     B    R      4  4  1      3  3  0       3846.98903    2.068E+00   0.5626
  0, 5000
        TOTAL BAND INTENSITY(GAUSSIAN SUM) = 4.9228E+01

        MAXIMUM INTENSITY = 1.3810E+00
```

```fortran
C
C       PROGRAM ASYMABS.FOR
C
        IMPLICIT REAL*8(A-H,O-Z)
C
C       ASYMMETRIC ROTOR FREQUENCY ESTIMATION PROGRAM
C       FOR INFRARED AND VISIBLE SPECTROSCOPY
C                                            CODED BY Y.E.
C
C            MODIFIED BY C.H.D.,R.T.L.,H.H.N.
C
C
        DIMENSION NAME(18),HD(50),HF(50),HDLO(50),HFLO(50),
     1           EL(50),ELLO(50),CFAC(50),CFACP(50),TVF(50),
     2           TVI(50),LTYPE(3),P(30)
        LOGICAL LTYPE
        COMMON /CON/ PAR(30)
        COMMON /FREQ/ FMIN,FMAX
        COMMON/BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH
        COMMON/OTPUT/ACCES1$
        COMMON/INTEN/TOTINT,STRENGTH
        CHARACTER*24 ACCESS$,ACCES1$
        CHARACTER*8 FILENM$,FILNM1$
        INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
        CALL GETTIM(IHOUR,IMINUTE)
        CALL GETDAT(IYEAR,IMONTH,IDAY)
C
C
C       ENTER NAME OF PARAMETER FILE TO BE USED AS INPUT
C
        WRITE (6,*) 'ENTER INPUT FILE NAME?'
        READ 99,FILENM$
99      FORMAT(A8)
C
C       ENTER NAME OF FILE TO BE USED FOR STORAGE OF OUTPUT
C
        WRITE (6,*) 'ENTER OUTPUT FILE NAME?'
        READ 99,FILNM1$
C
C       THE INPUT PARAMETER FILE IS LOCATED ON DRIVE C: IN
C       SUBDIRECTORY ASYMRTR
C
C       THE OUTPUT FILE IS WRITTEN TO DRIVE A:
C
        ACCESS$ = 'C:\ASYMRTR\'//FILENM$//'.DAT'
        ACCES1$ = 'A:'//FILNM1$//'.DAT'
        OPEN (2,FILE=ACCESS$,ACCESS='SEQUENTIAL')
C
C       ISOTOPE CODE IS READ:
C             161 = H2O
C             262 = D2O
C             162 = HDO
C
```

```
         READ(2,*) ISOTOPE
C
C        THE VARIABLES ARE READ FROM THE PARAMETER FILE:
C             PAR(1,2,3) = A,B,C VALUES FOR THE UPPER STATE
C             PAR(4,5,6,7,8) = CENTRIFUGAL DISTORTION CONSTANTS
C                 FOR THE UPPER STATE
C             PAR(10-15) = UNUSED IN PRESENT VERSION; ALL = 0
C             PAR(16,17,18) = A,B,C VALUES FOR THE LOWER STATE
C             PAR(19,20,21,22,23) = CENTRIFUGAL DISTORTION
C                 CONSTANTS FOR THE LOWER STATE
C             PAR(24-30) = UNUSED IN PRESENT VERSION; ALL = 0
C
         DO 111 I=1,7,3
111      READ(2,*) (PAR(J), J=I,I+2)
67       FORMAT(3F16.8)
         DO 121  I=10,15
121      PAR(I)=0.
         DO 131 I=16,22,3
131      READ(2,*) (PAR(J), J=I,I+2)
         DO 141 I=25,30
141      PAR(I)=0.
C
C        READ NBINS = NUMBER OF BINS INTO WHICH FREQUENCY RANGE IS
C        DIVIDED AND WIDTH = HALF-WIDTH OF GAUSSIAN LINE SHAPE
C
         READ (2,84) NBINS,WIDTH
84       FORMAT (I5,F10.6)
C
C        READ IITY = BAND TYPE
C             100 = A TYPE BAND
C             010 = B TYPE BAND
C             001 = C TYPE BAND
C        JMIN AND JMAX SET MINIMUM AND MAXIMUM VALUES OF J
C        KTAU = MAXIMUM CHANGE ALLOWED IN TAU
C
         READ (2,69) IITY,JMIN,JMAX,KTAU
69       FORMAT (4I4)
C
C        FMIN AND FMAX SET ALLOWED LIMITS FOR FREQUENCY RANGE
C        IN CM-1. FNUZ IS THE BAND CENTER IN CM-1
C
         READ (2,79) FMIN,FMAX,FNUZ
C
C        STMIN = MINIMUM STRENGTH FOR STORAGE OF LINE
C        TT = TEMPERATURE
C        BS = BAND STRENGTH FOR TRANSITION BEING CALCULATED
C
         READ(2,59) STMIN,TT,BS
59       FORMAT(E12.3,2F10.4)
C
C        FNU1,FNU2,FNU3 ARE THE FUNDAMENTAL FREQUENCIES IN CM-1
C
         READ (2,79) FNU1,FNU2,FNU3
```

```
79      FORMAT(3F10.4)
        CLOSE (2)
C
C       THE PARAMETERS READ FROM THE PARAMETER FILE ARE
C       PRINTED OUT.
C
        WRITE (6,6019)
6019    FORMAT (10X,'OUTPUT FROM PROGRAM ASYMABS.FOR'///)
        WRITE(6,6022) IMONTH,IDAY,IYEAR
6022    FORMAT(1X,I2,'/',I2,'/',I4)
        WRITE(6,6023) IHOUR,IMINUTE
6023    FORMAT(1X,I2,':',I2/)
        WRITE(6,6034) FILENM$
        WRITE(6,6036) FILNM1$
        WRITE(6,6029) ISOTOPE
6029    FORMAT(' ISOTOPE =',I4//)
6034    FORMAT(' PARAMETER FILE = ',A8//) .
6036    FORMAT(' OUTPUT FILE = ',A8//)
        WRITE(6,6020) (PAR(I), I=1,8)
6020    FORMAT(' UPPER STATE CONSTANTS'//
       1            ' A   =',F16.4,5X,'B   =',F16.4,5X,'C   =',F16.4/
       2            ' DLJ =',F16.8,5X,'DLJK=',F16.8,5X,'DLK =',F16.8/
       3            ' DSJ =',F16.8,5X,'DSK =',F16.8//)
        WRITE (6,6025) (PAR(I), I=16,23)
6025    FORMAT(' LOWER STATE CONSTANTS'//
       1            ' A   =',F16.4,5X,'B   =',F16.4,5X,'C   =',F16.4/
       2            ' DLJ =',F16.8,5X,'DLJK=',F16.8,5X,'DLK =',F16.8/
       3            ' DSJ =',F16.8,5X,'DSK =',F16.8//)
        DO 100 I=1,3
100     LTYPE(I)=.FALSE.
        IF (IITY.GE.100)  LTYPE(1)=.TRUE.
        IF (MOD(IITY,100).GE.10) LTYPE(2)=.TRUE.
        IF (MOD(IITY,10) .GE. 1) LTYPE(3)=.TRUE.
        WRITE(6,6030)  LTYPE,JMIN,JMAX
6030    FORMAT(//' SELECTION RULES  ',3L4/
       1            ' J RANGE  ',I4,' TO ',I4)
        WRITE(6,6040)  KTAU,FMIN,FMAX,FNUZ,FNU1,FNU2,FNU3,
       1            STMIN,TT,NBINS,WIDTH,BS
6040    FORMAT(//' MAX. DELTA  TAU  ',I4/
       1             ' FREQ. RANGE          ',F10.4,' TO ',F10.4,' CM-1'
       2             ' BAND ORIGIN          ',F10.4,' CM-1'/
       7             ' NU #1                ',F10.4,' CM-1'/
       8             ' NU #2                ',F10.4,' CM-1'/
       9             ' NU #3                ',F10.4,' CM-1'/
       3             ' MIN. STRENGTH    ',E12.3/
       4             ' TEMPERATURE      ',F7.2/
       5             ' NBINS            ',I5/
       6             ' WIDTH            ',F10.6/
       7                 ' BAND STRENGTH    ',F10.4///)
C
C
C       SET LINE COUNTER TO ZERO
C
```

```
         NLINE = 0
C
C        SET INITIAL TOTAL BAND INTENSITY = 0
C
         TOTINT=0.0
C
C        DEFINE FCT = FACTOR FOR BOLTZMANN CALCULATIONS
C
         FCT=-1.438786/TT
C
C        CALCULATE VIBRATIONAL PARTITION FUNCTION
C
         VIBPF=1./((1.-DEXP(FCT*FNU1))*(1.-DEXP(FCT*FNU2))*
     1          (1.-DEXP(FCT*FNU3)))
C
C        CALCULATE ROTATIONAL PARTITION FUNCTION
C
         ROTPF=(TT**3/(PAR(16)*PAR(17)*PAR(18)))**.5
C
C
         DO 9000 J=JMIN,JMAX
C
C        PRINT J ON SCREEN TO TRACK PROGRESS OF CALCULATION
C
         PRINT 6010,J
6010     FORMAT (1X,I5)
C
C
C****** R BRANCH TRANSITIONS
C
         IF (J.EQ.JMIN)  GO TO 4000
         FLJIN=1.D0/DBLE(J)
         JLO  = J-1
C
         DO 2000 NTYPE=1,3
         IF (.NOT.LTYPE(NTYPE))  GO TO 2000
C
C
         DO 2100 ISYMF=1,4
C
         ISYMI = ISEL(ISYMF,NTYPE,1)
         CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
         CALL ECALC(1,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
         IF (NHF*NHI.EQ.0)  GO TO 2100
C
C****** CALCULATE DIRECTION COSINE
C
         CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C****** RANGE OF ISHIFT
C
         NTDEL = MAXT-MAXTLO
         NSMAX = (KTAU-NTDEL+100)/4-25
```

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```
              NSMIN = 25-(KTAU+NTDEL+100)/4
C
C

       DO 2200 ISHIFT=NSMIN,NSMAX
       IF (ISHIFT.GE.0)   GO TO 2180
       N = MINO(NHF+ISHIFT,NHI)
       IF (N.LT.1)  GO TO 2200
       NPLUSF = -ISHIFT
       NPLUSI = 0
       GO TO 2210
C
2180   N = MINO(NHF,NHI-ISHIFT)
       IF (N.LT.1)  GOTO 2200
       NPLUSF = 0
       NPLUSI = ISHIFT
2210   CONTINUE
C
C****** CALCULATE INDIVIDUAL TRANSITIONS
C
       DO 2300 I=1,N
       INOF = I+NPLUSF
       INOI = I+NPLUSI
       ELF  = EL(INOF)
       ELI  = ELLO(INOI)
       FREQ = (ELF-ELI)/1.+FNUZ
C
C      TEST WHETHER LINE POSITION IS WITHIN SPECIFIED
C      FREQUENCY RANGE. IF SO, CONTINUE WITH INTENSITY
C      CALCULATION; IF NOT,CALCULATE NEXT LINE.
C
       IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)   GO TO 2300
C
C****** LEVEL NAMES
C
       KAF = KMAXF+2*(1-INOF)
       KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
       KAI = KMAXI+2*(1-INOI)
       KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
C****** CALCULATE EIGEN VECTORS
C
       CALL EIVEC(NHF,HD,HF,ELF,TVF)
       CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** CALCULATE LINE STRENGTH
C
       FAC = 0.0D0
       IPLUS = 0
       IF (KMAXF-KMAXI.EQ.2)   IPLUS = 1
       NN = MINO(NHF-IPLUS,NHI)
       DO 2520 II=1,NN
2520   FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
       IF (NTYPE.EQ.1)   GOTO 2540
```

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```
          FACP = 0.0D0
          NN = MIN0(NHF-1,NHI)
          IF (NN.LT.1)  GO TO 2512
          DO 2530 II=1,NN
2530      FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
2512      IF (NTYPE.EQ.2)  FACP = -FACP
          FAC = FAC+FACP
2540      STRE = FAC**2*FLJIN
C
C         MULTIPLY DIRECTION COSINES FACTOR BY ROTATIONAL BOLTZMANN
C         FACTOR OVER ROTATIONAL PARTITION FUNCTION
C
          STRE=(STRE*DEXP(-ELI/(0.695*TT)))/ROTPF
C
C         ASSIGN NUCLEAR STATISTICS FACTOR BASED ON IDENTITY OF
C         ISOTOPE AND WHETHER LEVEL IS ODD OR EVEN
C              H2O    1:3 FOR EVEN:ODD
C              D2O    6:3 FOR EVEN:ODD
C              HDO    1 FOR ALL LEVELS
C
          KK=IABS(KAI-KCI)
          IF(ISOTOPE.EQ.161) THEN
          STNUC=(1.+2.*(REAL(MOD(KK,2))))
          ELSEIF(ISOTOPE.EQ.262) THEN
          STNUC=(6.-3.*(REAL(MOD(KK,2))))
          ELSE
          STNUC=1.0
          ENDIF
C
C         STIMULATED EMISSION CONTRIBUTION IS CALCULATED.
C
          STIMEM=(1.-DEXP(FCT*FREQ))
C
C         CALCULATE STRENGTH WHICH INCLUDES ROTATIONAL AND NUCLEAR
C         STATISTICS FACTORS.  THIS WILL BE USED LATER TO NORMALIZE
C         FOR COMPARISON OF DIFFERENT ISOTOPES. TOTINT IS SUM OF
C         STRENGTH FOR EACH LINE.
C
          STRENGTH=STNUC*STRE
C
C         CALCULATE FINAL INTENSITY BY MULTIPLYING BY THE INDUCED
C         EMISSION TERM, THE FREQUENCY,AND THE BAND STRENGTH AND
C         DIVIDING BY VIBRATIONAL PARTITION FUNCTION AND BAND CENTER.
C
          STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)
C
C****** STORE THE CALCULATED TRANSITION IF STRE EXCEEDS THE
C       MINIMUM STRENGTH CRITERION.
C
          IF (STRE.GE.STMIN) CALL STORE(NLINE,J,KAF,KCF,JLO,KAI,
         1                              KCI,FREQ,STRE,NTYPE)
2300      CONTINUE
2200      CONTINUE
```

```
2100    CONTINUE
2000    CONTINUE
C
C
C****** P BRANCH TRANSITIONS - P BRANCH TRANSITION FREQUENCIES
C       AND STRENGTHS ARE CALCULATED BY THE SAME METHOD USED
C       ABOVE FOR THE R BRANCH TRANSITIONS.
C
4000    CONTINUE
C
C
        IF (J.EQ.JMIN)  GO TO 4200
        FLJIN = 1.D0/DBLE(J)
        JLO   = J-1
C
C
        DO 3000 NTYPE=1,3
        IF (.NOT.LTYPE(NTYPE))  GO TO 3000
C
        DO 3100 ISYMF=1,4
        ISYMI = ISEL(ISYMF,NTYPE,1)
        CALL ECALC(1,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
        CALL ECALC(0,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
        IF (NHF*NHI.EQ.0)  GO TO 3100
C
C****** CALCULATE DIRECTION COSINES
C
        CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C****** RANGE OF ISHIFT
C
        NTDEL = MAXT-MAXTLO
        NSMAX = (KTAU-NTDEL+100)/4-25
        NSMIN = 25-(KTAU+NTDEL+100)/4
C
C
        DO 3200 ISHIFT=NSMIN,NSMAX
        IF (ISHIFT.GE.0)  GO TO 3180
        N = MIN0(NHF+ISHIFT,NHI)
        IF (N.LT.1)  GOTO 3200
        NPLUSF = -ISHIFT
        NPLUSI = 0
        GOTO 3210
C
3180    N = MIN0(NHF,NHI-ISHIFT)
        IF (N.LT.1)  GOTO 3200
        NPLUSF = 0
        NPLUSI = ISHIFT
3210    CONTINUE
C
C****** CALCULATE INDIVIDUAL TRANSITIONS
C
        DO 3300 I=1,N
```

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```
              INOF = I+NPLUSF
              INOI = I+NPLUSI
              ELF  = EL(INOF)
              ELI  = ELLO(INOI)
              FREQ = (ELI-ELF)/1.+FNUZ
              IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)   GO TO 3300
C
C****** LEVEL NAMES
C
              KAF = KMAXF+2*(1-INOF)
              KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
              KAI = KMAXI+2*(1-INOI)
              KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
C****** CALCULATE EIGEN VECTORS
C
              CALL EIVEC(NHF,HD,HF,ELF,TVF)
              CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** CALCULATE LINE STRENGTH
C
              FAC = 0.0D0
              IPLUS = 0
              IF (KMAXF-KMAXI.EQ.2)   IPLUS = 1
              NN = MINO(NHF-IPLUS,NHI)
              DO 3520 II=1,NN
 3520    FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
              IF (NTYPE.EQ.1)   GOTO 3540
              FACP = 0.0D0
              NN = MINO(NHF-1,NHI)
              IF (NN.LT.1)   GO TO 3512
              DO 3530 II=1,NN
 3530    FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
 3512    IF (NTYPE.EQ.2)   FACP = -FACP
              FAC = FAC+FACP
 3540    STRE = FAC**2*FLJIN
              STRE=(STRE*DEXP(-ELI/(0.695*TT)))/ROTPF
              KK=IABS(KAI-KCI)
              IF(ISOTOPE.EQ.161) THEN
              STNUC=(1.+2.*(REAL(MOD(KK,2))))
              ELSEIF(ISOTOPE.EQ.262) THEN
              STNUC=(6.-3.*(REAL(MOD(KK,2))))
              ELSE
              STNUC=1.0
              ENDIF
              STIMEM=(1.-DEXP(FCT*FREQ))
              STRENGTH=STNUC*STRE
              STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)
C
C****** STORE THE CALCULATED TRANSITION
C
              IF (STRE.GE.STMIN) CALL STORE(NLINE,JLO,KAI,KCI,J,KAF,
       1                                    KCF,FREQ,STRE,NTYPE)
```

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```
C
3300    CONTINUE
3200    CONTINUE
3100    CONTINUE
3000    CONTINUE
C
C
4100    CONTINUE
C
C
C****** Q BRANCH TRANSITIONS - Q BRANCH TRANSITION FREQUENCIES
C      AND LINE STRENGTHS ARE CALCULATED BY THE SAME METHOD
C      USED ABOVE FOR THE P AND R BRANCHES.
C
        IF (J.EQ.0)  GO TO 4200
        FLJIN = DBLE(J+J+1)/DBLE(J*(J+1))
C
C
        DO 7000 NTYPE=1,3
        IF (.NOT.LTYPE(NTYPE))  GO TO 7000
C
C
        DO 7100 ISYMF=1,4
        ISYMI = ISEL(ISYMF,NTYPE,0)
        CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
        CALL ECALC(1,ISYMI,J,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
        IF (NHF*NHI.EQ.0)  GO TO 7100
C
C******CALCULATE DIRECTION COSINES
C
        CALL CFACTR(0,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C****** RANGE OF ISHIFT
C
        NTDEL = MAXT-MAXTLO
        NSMAX = (KTAU-NTDEL+100)/4-25
        NSMIN = 25-(KTAU+NTDEL+100)/4
C
C
        DO 7200 ISHIFT=NSMIN,NSMAX
C
        IF (ISHIFT.GE.0)  GO TO 7320
        N = MINO(NHF+ISHIFT,NHI)
        IF (N.LT.1)  GO TO 7200
        NPLUSF = -ISHIFT
        NPLUSI = 0
        GO TO 7330
C
7320    N = MINO(NHF,NHI-ISHIFT)
        IF (N.LT.1)  GO TO 7200
        NPLUSF = 0
        NPLUSI = ISHIFT
C
```

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```
C****** INDIVIDUAL TRANSITIONS
C
7330  DO 7300 I=1,N
      INOF = I+NPLUSF
      INOI = I+NPLUSI
      ELF  = EL(INOF)
      ELI  = ELLO(INOI)                    ▲
      FREQ = (ELF-ELI)/1.+FNUZ
      IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)  GO TO 7300
C
C****** LEVEL NAMES
C
      KAF = KMAXF+2*(1-INOF)
      KCF = J+1-KAF-MOD(ISYMF,2)
      KAI = KMAXI+2*(1-INOI)
      KCI = J+1-KAI-MOD(ISYMI,2)
C
C******EIGEN VECTORS
C
      CALL EIVEC(NHF,HD,HF,ELF,TVF)
      CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C******LINE STRENGTH
C
      FAC = 0.0D0
      NN  = MIN0(NHI,NHF)
      DO 7520 II=1,NN
7520  FAC = FAC+CFAC(II)*TVF(II)*TVI(II)
      IF (NTYPE.EQ.1)  GO TO 7540
C
      FACP = 0.0D0
      IF (KMAXF.LT.J)  GO TO 7510
      NN  = MIN0(NHF-1,NHI)
      IF (NN.LT.1)  GO TO 7512
      DO 7514 II=1,NN
7514  FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
      GOTO 7512
C
7510  NN  = MIN0(NHF,NHI-1)
      IF (NN.LT.1)  GO TO 7512
      DO 7516 II=1,NN
7516  FACP = FACP+CFACP(II)*TVF(II)*TVI(II+1)
C
7512  IF (NTYPE.EQ.3)  FACP = -FACP
      FAC = FAC+FACP
C
7540  STRE = FAC**2*FLJIN
      STRE=(STRE*DEXP(-ELI/(0.695*TT)))/ROTPF
      KK=IABS(KAI-KCI)
      IF(ISOTOPE.EQ.161) THEN
      STNUC=(1.+2.*(REAL(MOD(KK,2))))
      ELSEIF(ISOTOPE.EQ.262) THEN
      STNUC=(6.-3.*(REAL(MOD(KK,2))))
```

```
         ELSE
         STNUC=1.0
         ENDIF
         STIMEM=(1.-DEXP(FCT*FREQ))
         STRENGTH=STNUC*STRE
         STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)
C
C******STORE THE CALCULATED TRANSITION
C
         IF (STRE.GE.STMIN)   CALL STORE(NLINE,J,KAF,KCF,J,KAI,
       1                                 KCI,FREQ,STRE,NTYPE)
C
7300     CONTINUE
7200     CONTINUE
7100     CONTINUE
7000     CONTINUE
C
C
4200     CONTINUE
C
C
C
9000     CONTINUE
C
C
C****** SORT AND PRINTOUT THE CALCULATED SPECTRUM
C
C        PRINT OUT THE TOTAL NUMBER OF LINES MEETING THE STRENGTH
C        AND FREQUENCY RANGE CRITERIA.
C
         WRITE(6,6013) NLINE
6013     FORMAT(10X,'TOTAL NUMBER OF LINES = ',I6/)
C
C        ARRANGE THE STORED TRANSITIONS IN ORDER OF INCREASING
C        FREQUENCY.
C
         CALL SORT(NLINE)
C
C        PRINT OUT THE TRANSITION TYPE AND QUANTUM STATE LABELS,
C        THE TRANSITION FREQUENCY, THE LINE STRENGTH AND
C        THE RELATIVE STRENGTH. DISABLE THIS SUBROUTINE CALL TO
C        SUPPRESS PRINTING.
C
C        CALL PRINT(NLINE)
C
C        PRINT OUT THE SUM OF STRENGTH WHICH INCLUDES ONLY THE
C        DIRECTION COSINE AND THE ROTATIONAL TERMS.
C
         WRITE (6,6017) TOTINT
6017     FORMAT(10X,'TOTAL BAND INTENSITY = ',1PE10.4/)
C
C        SORT THE STORED TRANSITIONS INTO FREQUENCY BINS OF WIDTH
C        EQUAL TO THE FREQUENCY RANGE DIVIDED BY NBINS.
```

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```
C
        CALL BINSORT(NLINE)
C
C       APPLY A GAUSSIAN LINE SHAPE OF HALFWIDTH = "WIDTH" TO THE
C       SUMMED INTENSITY IN EACH BIN.
C
        CALL SHAPE(NLINE)
C
        STOP
        END
```

```fortran
C
C       PROGRAM ASYMEMS.FOR
C
        IMPLICIT REAL*8(A-H,O-Z)
C
C       ASYMMETRIC ROTOR FREQUENCY ESTIMATION PROGRAM
C       FOR INFRARED AND VISIBLE SPECTROSCOPY
C                                           CODED BY Y.E.
C
C            MODIFIED BY C.H.D.,R.T.L.,H.H.N.
C
C
        DIMENSION NAME(18),HD(50),HF(50),HDLO(50),HFLO(50),
     1            EL(50),ELLO(50),CFAC(50),CFACP(50),TVF(50),
     2            TVI(50),LTYPE(3),P(30)
        LOGICAL LTYPE
        COMMON /CON/ PAR(30)
        COMMON /FREQ/ FMIN,FMAX
        COMMON/BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH
        COMMON/OTPUT/ACCES1$
        COMMON/INTEN/TOTINT,STRENGTH
        CHARACTER*24 ACCESS$,ACCES1$
        CHARACTER*8 FILENM$,FILNM1$
        INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
        CALL GETTIM(IHOUR,IMINUTE)
        CALL GETDAT(IYEAR,IMONTH,IDAY)
C
C
C       ENTER NAME OF PARAMETER FILE TO BE USED AS INPUT
C
        WRITE (6,*) 'ENTER INPUT FILE NAME?'
        READ 99,FILENM$
99      FORMAT(A8)
C
C       ENTER NAME OF FILE TO BE USED FOR STORAGE OF OUTPUT
C
        WRITE (6,*) 'ENTER OUTPUT FILE NAME?'
        READ 99,FILNM1$
C
C       THE INPUT PARAMETER FILE IS LOCATED ON DRIVE C: IN
C       SUBDIRECTORY ASYMRTR
C
C       THE OUTPUT FILE IS WRITTEN TO DRIVE A:
C
        ACCESS$ = 'C:\ASYMRTR\'//FILENM$//'.DAT'
        ACCES1$ = 'A:'//FILNM1$//'.DAT'
        OPEN (2,FILE=ACCESS$,ACCESS='SEQUENTIAL')
C
C       ISOTOPE CODE IS READ:
C            161 = H2O
```

```
C              262 = D2O
C              162 = HDO
C
      READ(2,*) ISOTOPE
C
C     THE VARIABLES ARE READ FROM THE PARAMETER FILE:
C          PAR(1,2,3) = A,B,C VALUES FOR THE UPPER STATE
C          PAR(4,5,6,7,8) = CENTRIFUGAL DISTORTION CONSTANTS
C               FOR THE UPPER STATE
C          PAR(10-15) = UNUSED IN PRESENT VERSION; ALL = 0
C          PAR(16,17,18) = A,B,C VALUES FOR THE LOWER STATE
C          PAR(19,20,21,22,23) = CENTRIFUGAL DISTORTION
C               CONSTANTS FOR THE LOWER STATE
C          PAR(24-30) = UNUSED IN PRESENT VERSION; ALL = 0
C
      DO 111 I=1,7,3
111   READ(2,*) (PAR(J), J=I,I+2)
67    FORMAT(3F16.8)
      DO 121  I=10,15
121   PAR(I)=0.
      DO 131 I=16,22,3
131   READ(2,*) (PAR(J), J=I,I+2)
      DO 141 I=25,30
141   PAR(I)=0.
C
C     READ NBINS = NUMBER OF BINS INTO WHICH FREQUENCY RANGE IS
C     DIVIDED AND WIDTH = HALF-WIDTH OF GAUSSIAN LINE SHAPE
C
      READ (2,84) NBINS,WIDTH
84    FORMAT (I5,F10.6)
C
C     READ IITY = BAND TYPE
C          100 = A TYPE BAND
C          010 = B TYPE BAND
C          001 = C TYPE BAND
C     JMIN AND JMAX SET MINIMUM AND MAXIMUM VALUES OF J
C     KTAU = MAXIMUM CHANGE ALLOWED IN TAU
C
      READ (2,69) IITY,JMIN,JMAX,KTAU
69    FORMAT (4I4)
C
C     FMIN AND FMAX SET ALLOWED LIMITS FOR FREQUENCY RANGE
C     IN CM-1. FNUZ IS THE BAND CENTER IN CM-1
C
      READ (2,79) FMIN,FMAX,FNUZ
58    FORMAT(3F10.6)
C
C     STMIN = MINIMUM STRENGTH FOR STORAGE OF LINE
C     TT = TEMPERATURE
C     BS = BAND STRENGTH FOR TRANSITION BEING CALCULATED
C
      READ(2,59) STMIN,TT,BS
59    FORMAT(E12.3,2F10.4)
```

```
C
C      FNU1,FNU2,FNU3 ARE THE FUNDAMENTAL FREQUENCIES IN CM-1
C
       READ (2,79) FNU1,FNU2,FNU3
79     FORMAT(3F10.4)
       CLOSE (2)
C
C      THE PARAMETERS READ FROM THE PARAMETER FILE ARE
C      PRINTED OUT.
C
       WRITE (6,6019)
6019   FORMAT (10X,'OUTPUT FROM PROGRAM ASYMEMS.FOR'////)
       WRITE(6,6022) IMONTH,IDAY,IYEAR
6022   FORMAT(1X,I2,'/',I2,'/',I4)
       WRITE(6,6023) IHOUR,IMINUTE
6023   FORMAT(1X,I2,':',I2/)
       WRITE(6,6034) FILENM$
       WRITE(6,6036) FILNM1$
       WRITE(6,6029) ISOTOPE
6029   FORMAT(' ISOTOPE =',I4//)
6034   FORMAT(' PARAMETER FILE = ',A8//)
6036   FORMAT(' OUTPUT FILE = ',A8//)
       WRITE(6,6020) (PAR(I), I=1,8)
6020   FORMAT(' UPPER STATE CONSTANTS'//
      1          ' A   =',F16.4,5X,'B   =',F16.4,5X,'C   =',F16.4/
      2          ' DLJ =',F16.8,5X,'DLJK=',F16.8,5X,'DLK =',F16.8/
      3          ' DSJ =',F16.8,5X,'DSK =',F16.8//)
       WRITE (6,6025) (PAR(I), I=16,23)
6025   FORMAT(' LOWER STATE CONSTANTS'//
      1          ' A   =',F16.4,5X,'B   =',F16.4,5X,'C   =',F16.4/
      2          ' DLJ =',F16.8,5X,'DLJK=',F16.8,5X,'DLK =',F16.8/
      3          ' DSJ =',F16.8,5X,'DSK =',F16.8//)
       DO 100 I=1,3
100    LTYPE(I)=.FALSE
       IF (IITY.GE.100)   LTYPE(1)=.TRUE.
       IF (MOD(IITY,100).GE.10) LTYPE(2)=.TRUE.
       IF (MOD(IITY,10) .GE. 1) LTYPE(3)=.TRUE.
       WRITE(6,6030)   LTYPE,JMIN,JMAX
6030   FORMAT(//' SELECTION RULES  ',3L4/
      1          ' J RANGE  ',I4,' TO ',I4)
       WRITE(6,6040)   KTAU,FMIN,FMAX,FNUZ,FNU1,FNU2,FNU3,
      1          STMIN,TT,NBINS,WIDTH,BS
6040   FORMAT(//' MAX. DELTA  TAU ',I4/
      1          ' FREQ. RANGE       ',F10.4,' TO ',F10.4,' CM-1'
      2          ' BAND ORIGIN       ',F10.4,' CM-1'/
      7          ' NU #1             ',F10.4,' CM-1'/
      8          ' NU #2             ',F10.4,' CM-1'/
      9          ' NU #3             ',F10.4,' CM-1'/
      3          ' MIN. STRENGTH     ',E12.3/
      4          ' TEMPERATURE       ',F7.2/
      5          ' NBINS             ',I5/
      6          ' WIDTH             ',F10.6/
      7              ' BAND STRENGTH     ',F10.4///)
```

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```
C
C
C        SET LINE COUNTER TO ZERO
C
         NLINE = 0
C
C        SET INITIAL TOTAL BAND INTENSITY = 0
C
         TOTINT=0.0
C
C        DEFINE FCT = FACTOR FOR BOLTZMANN CALCULATIONS
C
         FCT=-1.438786/TT
C
C        CALCULATE VIBRATIONAL PARTITION FUNCTION
C
         VIBPF=1./((1.-DEXP(FCT*FNU1))*(1.-DEXP(FCT*FNU2))*
        1        (1.-DEXP(FCT*FNU3)))
C
C        CALCULATE ROTATIONAL PARTITION FUNCTION
C
         ROTPF=(TT**3/(PAR(16)*PAR(17)*PAR(18)))**.5
C
C
         DO 9000 J=JMIN,JMAX
C
C        PRINT J ON SCREEN TO TRACK PROGRESS OF CALCULATION
C
         PRINT 6010,J
6010     FORMAT (1X,I5)
C
C
C****** R BRANCH TRANSITIONS
C
         IF (J.EQ.JMIN)  GO TO 4000
         FLJIN=1.D0/DBLE(J)
         JLO  = J-1
C
         DO 2000 NTYPE=1,3
         IF (.NOT.LTYPE(NTYPE))  GO TO 2000
C
C
         DO 2100 ISYMF=1,4
C
         ISYMI = ISEL(ISYMF,NTYPE,1)
         CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
         CALL ECALC(1,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
         IF (NHF*NHI.EQ.0)  GO TO 2100
C
C****** CALCULATE DIRECTION COSINE
C
         CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
```

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```
C****** RANGE OF ISHIFT
C
      NTDEL = MAXT-MAXTLO
      NSMAX = (KTAU-NTDEL+100)/4-25
      NSMIN = 25-(KTAU+NTDEL+100)/4
C
C
      DO 2200 ISHIFT=NSMIN,NSMAX
      IF (ISHIFT.GE.0)  GO TO 2180
      N = MIN0(NHF+ISHIFT,NHI)
      IF (N.LT.1)  GO TO 2200
      NPLUSF = -ISHIFT
      NPLUSI = 0
      GO TO 2210
C
2180  N = MIN0(NHF,NHI-ISHIFT)
      IF (N.LT.1)  GOTO 2200
      NPLUSF = 0
      NPLUSI = ISHIFT
2210  CONTINUE
C
C****** CALCULATE INDIVIDUAL TRANSITIONS
C
      DO 2300 I=1,N
      INOF = I+NPLUSF
      INOI = I+NPLUSI
      ELF  = EL(INOF)
      ELI  = ELLO(INOI)
      FREQ = (ELF-ELI)/1.+FNUZ
C
C     TEST WHETHER LINE POSITION IS WITHIN SPECIFIED FREQUENCY
C     RANGE. IF SO, CONTINUE WITH INTENSITY CALCULATION;
C     IF NOT, CALCULATE NEXT LINE.
C
      IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)  GO TO 2300
C
C****** LEVEL NAMES
C
      KAF = KMAXF+2*(1-INOF)
      KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
      KAI = KMAXI+2*(1-INOI)
      KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
C****** CALCULATE EIGEN VECTORS
C
      CALL EIVEC(NHF,HD,HF,ELF,TVF)
      CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** CALCULATE LINE STRENGTH
C
      FAC = 0.0D0
      IPLUS = 0
      IF (KMAXF-KMAXI.EQ.2)  IPLUS = 1
```

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```
          NN = MIN0(NHF-IPLUS,NHI)
          DO 2520 II=1,NN
2520   FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
          IF (NTYPE.EQ.1)   GOTO 2540
          FACP = 0.0D0
          NN = MIN0(NHF-1,NHI)
          IF (NN.LT.1)   GO TO 2512
          DO 2530 II=1,NN
2530   FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
2512   IF (NTYPE.EQ.2)   FACP = -FACP
          FAC = FAC+FACP
2540   STRE = FAC**2*FLJIN
C
C        MULTIPLY DIRECTION COSINES FACTOR BY ROTATIONAL BOLTZMANN
C        FACTOR OVER ROTATIONAL PARTITION FUNCTION
C
          STRE=(STRE*DEXP(-ELF/(0.695*TT)))/ROTPF
C
C        ASSIGN NUCLEAR STATISTICS FACTOR BASED ON IDENTITY OF
C        ISOTOPE AND WHETHER LEVEL IS ODD OR EVEN
C               H2O    1:3 FOR EVEN:ODD
C               D2O    6:3 FOR EVEN:ODD
C               HDO    1 FOR ALL LEVELS
C
          KK=IABS(KAF-KCF)
          IF(ISOTOPE.EQ.161) THEN
          STNUC=(1.+2.*(REAL(MOD(KK,2))))
          ELSEIF(ISOTOPE.EQ.262) THEN
          STNUC=(6.-3.*(REAL(MOD(KK,2))))
          ELSE
          STNUC=1.0
          ENDIF
C
C        STIMULATED EMISSION IS NOT USED IN EMISSION CALCULATION
C
C        STIMEM=(1.-DEXP(FCT*FREQ))
C
C        CALCULATE STRENGTH WHICH INCLUDES ROTATIONAL AND NUCLEAR
C        STATISTICS FACTORS.  THIS WILL BE USED LATER TO NORMALIZE
C        FOR COMPARISON OF DIFFERENT ISOTOPES. TOTINT IS SUM OF
C        STRENGTH FOR EACH LINE.
C
          STRENGTH=STNUC*STRE
C
C        CALCULATE FINAL INTENSITY BY MULTIPLYING BY FREQUENCY**4,
C        BAND STRENGTH, VIBRATIONAL BOLTZMANN FACTOR, AND DIVIDING
C        BY VIBRATIONAL PARTITION FUNCTION AND BAND CENTER.
C
          STRE=(STRENGTH*(FREQ**4)*BS*DEXP(-(FNUZ)/(0.695*TT))),
      1         (VIBPF*FNUZ)
C
C****** STORE THE CALCULATED TRANSITION IF STRE EXCEEDS THE
C        MINIMUM STRENGTH CRITERION.
```

```
C
      IF (STRE.GE.STMIN) CALL STORE(NLINE,J,KAF,KCF,JLO,KAI,
     1                                   KCI,FREQ,STRE,NTYPE)
2300  CONTINUE
2200  CONTINUE
2100  CONTINUE
2000  CONTINUE
C
C
C****** P BRANCH TRANSITIONS - P BRANCH TRANSITION FREQUENCIES
C      AND STRENGTHS ARE CALCULATED BY THE SAME METHOD USED
C      ABOVE FOR THE R BRANCH TRANSITIONS.
C
4000  CONTINUE
C
C
      IF (J.EQ.JMIN)  GO TO 4200
      FLJIN = 1.D0/DBLE(J)
      JLO   = J-1
C
C
      DO 3000 NTYPE=1,3
      IF (.NOT.LTYPE(NTYPE))  GO TO 3000
C
      DO 3100 ISYMF=1,4
      ISYMI = ISEL(ISYMF,NTYPE,1)
      CALL ECALC(1,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
      CALL ECALC(0,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
      IF (NHF*NHI.EQ.0)  GO TO 3100
C
C****** CALCULATE DIRECTION COSINES
C
      CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C****** RANGE OF ISHIFT
C
      NTDEL = MAXT-MAXTLO
      NSMAX = (KTAU-NTDEL+100)/4-25
      NSMIN = 25-(KTAU+NTDEL+100)/4
C
C
      DO 3200 ISHIFT=NSMIN,NSMAX
      IF (ISHIFT.GE.0)  GO TO 3180
      N = MINO(NHF+ISHIFT,NHI)
      IF (N.LT.1)  GOTO 3200
      NPLUSF = -ISHIFT
      NPLUSI = 0
      GOTO 3210
C
3180  N = MINO(NHF,NHI-ISHIFT)
      IF (N.LT.1)  GOTO 3200
      NPLUSF = 0
      NPLUSI = ISHIFT
```

40

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3210  CONTINUE
C
C****** CALCULATE INDIVIDUAL TRANSITIONS
C
      DO 3300 I=1,N
      INOF = I+NPLUSF
      INOI = I+NPLUSI
      ELF  = EL(INOF)
      ELI  = ELLO(INOI)
      FREQ = (ELI-ELF)/1.+FNUZ
      IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)  GO TO 3300
C
C****** LEVEL NAMES
C
      KAF = KMAXF+2*(1-INOF)
      KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
      KAI = KMAXI+2*(1-INOI)
      KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
C****** CALCULATE EIGEN VECTORS
C
      CALL EIVEC(NHF,HD,HF,ELF,TVF)
      CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** CALCULATE LINE STRENGTH
C
      FAC = 0.0D0
      IPLUS = 0
      IF (KMAXF-KMAXI.EQ.2)  IPLUS = 1
      NN = MIN0(NHF-IPLUS,NHI)
      DO 3520 II=1,NN
3520  FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
      IF (NTYPE.EQ.1)  GOTO 3540
      FACP = 0.0D0
      NN = MIN0(NHF-1,NHI)
      IF (NN.LT.1)  GO TO 3512
      DO 3530 II=1,NN
3530  FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
3512  IF (NTYPE.EQ.2)  FACP = -FACP
      FAC = FAC+FACP
3540  STRE = FAC**2*FLJIN
      STRE=(STRE*DEXP(-ELF/(0.695*TT)))/ROTPF
      KK=IABS(KAF-KCF)
      IF(ISOTOPE.EQ.161) THEN
      STNUC=(1.+2.*(REAL(MOD(KK,2))))
      ELSEIF(ISOTOPE.EQ.262) THEN
      STNUC=(6.-3.*(REAL(MOD(KK,2))))
      ELSE
      STNUC=1.0
      ENDIF
C     STIMEM=(1.-DEXP(FCT*FREQ))
      STRENGTH=STNUC*STRE
      STRE=(STRENGTH*(FREQ**4)*BS*DEXP(-(FNUZ)/(0.695*TT)))/
```

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      1          (VIBPF*FNUZ)
C
C****** STORE THE CALCULATED TRANSITION
C
      IF (STRE.GE.STMIN) CALL STORE(NLINE,JLO,KAI,KCI,J,KAF,
     1                              KCF,FREQ,STRE,NTYPE)
C
3300  CONTINUE
3200  CONTINUE
3100  CONTINUE
3000  CONTINUE
C
C
4100  CONTINUE
C
C
C****** Q BRANCH TRANSITIONS -.Q BRANCH TRANSITION FREQUENCIES
C      AND LINE STRENGTHS ARE CALCULATED BY THE SAME METHOD
C      USED ABOVE FOR THE P AND R BRANCHES.
C
      IF (J.EQ.0)   GOTO 4200
      FLJIN = DBLE(J+J+1)/DBLE(J*(J+1))
C
C
      DO 7000 NTYPE=1,3
      IF (.NOT.LTYPE(NTYPE))   GO TO 7000
C
C
      DO 7100 ISYMF=1,4
      ISYMI = ISEL(ISYMF,NTYPE,0)
      CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
      CALL ECALC(1,ISYMI,J,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
      IF (NHF*NHI.EQ.0)   GO TO 7100
C
C******CALCULATE DIRECTION COSINES
C
      CALL CFACTR(0,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C****** RANGE OF ISHIFT
C
      NTDEL = MAXT-MAXTLO
      NSMAX = (KTAU-NTDEL+100)/4-25
      NSMIN = 25-(KTAU+NTDEL+100)/4
C
C
      DO 7200 ISHIFT=NSMIN,NSMAX
C
      IF (ISHIFT.GE.0)   GO TO 7320
      N = MINO(NHF+ISHIFT,NHI)
      IF (N.LT.1)   GO TO 7200
      NPLUSF = -ISHIFT
      NPLUSI = 0
      GO TO 7330
```

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```
C
7320  N = MIN0(NHF,NHI-ISHIFT)
      IF (N.LT.1)  GO TO 7200
      NPLUSF = 0
      NPLUSI = ISHIFT
C
C****** INDIVIDUAL TRANSITIONS
C
7330  DO 7300 I=1,N
      INOF = I+NPLUSF
      INOI = I+NPLUSI
      ELF  = EL(INOF)
      ELI  = ELLO(INOI)
      FREQ = (ELF-ELI)/1.+FNUZ
      IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN)  GO TO 7300
C
C****** LEVEL NAMES
C
      KAF = KMAXF+2*(1-INOF)
      KCF = J+1-KAF-MOD(ISYMF,2)
      KAI = KMAXI+2*(1-INOI)
      KCI = J+1-KAI-MOD(ISYMI,2)
C
C******EIGEN VECTORS
C
      CALL EIVEC(NHF,HD,HF,ELF,TVF)
      CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C******LINE STRENGTH
C
      FAC = 0.0D0
      NN  = MIN0(NHI,NHF)
      DO 7520 II=1,NN
7520  FAC = FAC+CFAC(II)*TVF(II)*TVI(II)
      IF (NTYPE.EQ.1)  GO TO 7540
C
      FACP = 0.0D0
      IF (KMAXF.LT.J)  GO TO 7510
      NN  = MIN0(NHF-1,NHI)
      IF (NN.LT.1)  GO TO 7512
      DO 7514 II=1,NN
7514  FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
      GOTO 7512
C
7510  NN  = MIN0(NHF,NHI-1)
      IF (NN.LT.1)  GO TO 7512
      DO 7516 II=1,NN
7516  FACP = FACP+CFACP(II)*TVF(II)*TVI(II+1)
C
7512  IF (NTYPE.EQ.3)  FACP = -FACP
      FAC = FAC+FACP
C
7540  STRE = FAC**2*FLJIN
```

43

```fortran
      STRE=(STRE*DEXP(-ELF/(0.695*TT)))/ROTPF
      KK=IABS(KAF-KCF)
      IF(ISOTOPE.EQ.161) THEN
      STNUC=(1.+2.*(REAL(MOD(KK,2))))
      ELSEIF(ISOTOPE.EQ.262) THEN
      STNUC=(6.-3.*(REAL(MOD(KK,2))))
      ELSE
      STNUC=1.0
      ENDIF
C     STIMEM=(1.-DEXP(FCT*FREQ))
      STRENGTH=STNUC*STRE
      STRE=(STRENGTH*(FREQ**4)*BS*DEXP(-(FNUZ)/(0.695*TT)))/
     1      (VIBPF*FNUZ)
C******STORE THE CALCULATED TRANSITION
C
      IF (STRE.GE.STMIN)  CALL STORE(NLINE,J,KAF,KCF,J,KAI,
     1                                 KCI,FREQ,STRE,NTYPE)
C
7300  CONTINUE
7200  CONTINUE
7100  CONTINUE
7000  CONTINUE
C
C
4200  CONTINUE
C
C
9000  CONTINUE
C
C
C****** SORT AND PRINTOUT THE CALCULATED SPECTRUM
C
C     PRINT OUT THE TOTAL NUMBER OF LINES MEETING THE STRENGTH
C     AND FREQUENCY RANGE CRITERIA.
C
      WRITE(6,6013) NLINE
6013  FORMAT(10X,'TOTAL NUMBER OF LINES = ',I6/)
C
C     ARRANGE THE STORED TRANSITIONS IN ORDER OF INCREASING
C     FREQUENCY.
C
      CALL SORT(NLINE)
C
C     PRINT OUT THE TRANSITION TYPE AND QUANTUM STATE LABELS,
C     THE TRANSITION FREQUENCY, THE LINE STRENGTH AND THE
C     RELATIVE STRENGTH. DISABLE THIS SUBROUTINE CALL TO SUPPRESS
C     PRINTING.
C
C     CALL PRINT(NLINE)
C
C     PRINT OUT THE SUM OF STRENGTH WHICH INCLUDES ONLY THE
C     DIRECTION COSINE AND THE ROTATIONAL TERMS.
C
```

44

```
          WRITE (6,6017) TOTINT
6017      FORMAT(10X,'TOTAL BAND INTENSITY = ',1PE10.4/)
C
C         SORT THE STORED TRANSITIONS INTO FREQUENCY BINS OF WIDTH
C         EQUAL TO THE FREQUENCY RANGE DIVIDED BY NBINS.
C
          CALL BINSORT(NLINE)
C
C         APPLY A GAUSSIAN LINE SHAPE OF HALFWIDTH = "WIDTH" TO THE
C         SUMMED INTENSITY IN EACH BIN.
C
          CALL SHAPE(NLINE)
C
          STOP
          END
```

```
C
C       ASYMSUB.FOR
C
        INTEGER FUNCTION ISEL(ISYM,NTYPE,IQR)
C
C
        DIMENSION ITBL(4,3,2)
        DATA ITBL/ 2,1,4,3,   3,4,1,2,   4,3,2,1,
       1              1,2,3,4,   4,3,2,1,   3,4,1,2/
        ISEL = ITBL(ISYM,NTYPE,IQR+1)
        RETURN
        END
        SUBROUTINE CFACTR(IQR,NTYPE,NHF,NHI,KMAXF,KMAXI,J,
       1CFAC,CFACP)
        IMPLICIT REAL*8 (A-H,O-Z)
        DIMENSION CFAC(50),CFACP(50)
C
C       THIS ROUTINE CALCULATES THE DIRECTION COSINES
C           J NUMBER OF I STATE SHOULD BE LESS THAN OR EQUAL TO
C           THAT OF F STATE
C
        N = MIN0(NHF,NHI)
C
        IF (IQR.EQ.0)  GO TO 1000
C
C****** P,R BRANCH
C
        KP = KMAXI+2
        IF (NTYPE.NE.1)  GO TO 910
C
C****** A TYPE TRANSITION
C.
        JJ = J*J
        DO 920 I=1,N
        K  = KP-2*I
920     CFAC(I) = DSQRT(DBLE(JJ-K*K))
        RETURN
C
C****** B,C TYPE TRANSITIONS
C
910     DO 940 I=1,N
        K  = KP-2*I
        W  = (J+K)*(J+K+1)
        IF (K.EQ.0)  W = W+W
940     CFAC(I) = 0.5D0*DSQRT(W)
C
        N  = MIN0(NHF-1,NHI)
        IF (N.LE.0)  RETURN
        KP = KP-1
        DO 950 I=1,N
        K  = KP-2*I
        W  = (J-K)*(J-K-1)
        IF (K.EQ.0)  W = W+W
```

```
950    CFACP(I) = 0.5D0*DSQRT(W)
       RETURN
C
C****** Q BRANCH
C
1000   KP = KMAXF+2
       IF (NTYPE.NE.1)  GO TO 1160
C
C****** A TYPE TRANSITION
C
       DO 1170 I=1,N
1170   CFAC(I) = KP-2*I
       RETURN
C
C****** B,C TYPE TRANSITIONS
C
1160   JJ = J*(J+1)
       IF (KMAXF.LT.J)  GO TO 1190
       KP = KP-1
       NP = MIN0(NHF-1,NHI)
       GO TO 1165
1190   NP = MIN0(NHF,NHI-1)
C
1165   DO 1120 I=1,N
       K  = KP-2*I
       W  = JJ-K*(K+1)
       IF (K.EQ.0)  W = W+W
1120   CFAC(I) = 0.5D0*DSQRT(W)
C
       IF (NP.LT.1)  RETURN
       KP = KP-1
       DO 1125 I=1,NP
       K  = KP-2*I
       W  = JJ-K*(K+1)
       IF (K.EQ.0)  W = W+W
1125   CFACP(I) = 0.5D0*DSQRT(W)
       RETURN
       END
       SUBROUTINE ECALC(IUL,ISYM,J,HD,HF,EL,NH,KMX,MT)
       IMPLICIT REAL*8(A-H,O-Z)
       COMMON /CON/ PAR(30)     /CONST/ P(15)
       DIMENSION HD(50),HF(50),EL(50),HF1(50)
C
       IF (J.LE.98)  GO TO 100
       NH = 0
       RETURN
C
100    DO 110 I=1,15
110    P(I) = PAR(I+15*IUL)
C
C
       CALL MATRIX(ISYM,HD,HF,NH,KMX,J)
       IF (NH.EQ.0)  RETURN
```

```
                EL(NH)  = HD(NH)
                DO 200 I=1,NH-1
                HF1(I)  = HF(I)**2
                EL(I)   = HD(I)
200             CONTINUE
C
                IF (NH.NE.1)  CALL DTSM(NH,EL,HF1)
                MT = 3*J-ISYM+1-(J/2)*4
                IF (MT.GT.J)  MT = MT-4
                RETURN
                END
                SUBROUTINE STORE(NLINE,J,KAF,KCF,JL,KAI,KCI,FREQ,
               1STRE,NTYPE)
                IMPLICIT REAL*8(A-H,O-Z)
C
C       THIS ROUTINE STORES THE FREQUENCY, STRENGTH, AND LEVEL
C       NAME OF ALL TRANSITIONS MEETING THE STRENGTH AND
C       FREQUENCY RANGE CRITERIA.
C
                COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
                COMMON/INTEN/TOTINT,STRENGTH
C
C
C       THE LINE COUNTER NLINE IS ADVANCED AS EACH ADDITIONAL
C       LINE IS STORED.
C
                NLINE = NLINE+1
C
C       NO MORE THAN 10,000 LINES MAY BE STORED
C
                IF (NLINE.GT.10000) RETURN
                FRQ(NLINE) = FREQ
                ST(NLINE)  = STRE
                NLEV(NLINE)= ((J*100+KAF)*2+(KCF+KAF-J))*100000
               1             +((JL*100+KAI)*2+(KCI+KAI-JL))*5
               2             +NTYPE
C
C       STRENGTH IS SUMMED TO GIVE TOTINT.
C
                TOTINT=TOTINT+STRENGTH
                RETURN
                END
                SUBROUTINE SORT(NLINE)
C
C       THIS ROUTINE SORTS THE STORED TRANSITIONS BY FREQUENCY
C       AND STORES THEM AGAIN IN ORDER OF INCREASING WAVENUMBER.
C
                IMPLICIT REAL*8(A-H,O-Z)
                COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
                COMMON/INTEN/TOTINT,STRENGTH
C
                LOGNB2 = INT((ALOG(FLOAT(NLINE))/ALOG(2.0))+1.E-5)
                M=NLINE
```

```fortran
            DO 49 NN = 1,LOGNB2
            M=M/2
            K = NLINE - M
            DO 44 J = 1,K
            I = J
3     CONTINUE
            L = I+M
            IF (FRQ(L).LT.FRQ(I)) THEN
                F    =FRQ(I)
                S    =ST(I)
                N    =NLEV(I)
            FRQ(I)=FRQ(L)
            FRQ(L)=F
            ST(I)=ST(L)
            ST(L)=S
            NLEV(I)=NLEV(L)
            NLEV(L)=N
            I = I-M
            IF (I.GE.1) GOTO 3
            ENDIF
44          CONTINUE
49          CONTINUE
C
C     THIS LOOP NORMALIZES EACH ISOTOPE SO THAT THE SUM OF
C     TOTINT IS EQUAL TO 1. THIS IS DONE BY DIVIDING THE
C     STRENGTH OF EACH LINE BY TOTINT.
C
            DO 8005 I=1,NLINE
            ST(I)=ST(I)/TOTINT
8005        CONTINUE
            RETURN
            END
            SUBROUTINE PRINT(NLINE)
C
C     THIS ROUTINE PRINTS THE TRANSITION LABELS, FREQUENCY,
C     STRENGTH, AND RELATIVE STRENGTH FOR EACH LINE.
C
            IMPLICIT REAL*8(A-H,O-Z)
            COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
            DIMENSION INTYPE(3),ITYP(3)
            DATA INTYPE/1HA,1HB,1HC/,   ITYP/1HP,1HQ,1HR/
C
C
C     SMAX, USED TO CALCULATE RELATIVE STRENGTH, IS
CINITIALIZED TO 0.
C
            SMAX = 0.0D0
            DO 100 I=1,NLINE
            IF (SMAX.LT.ST(I))  SMAX=ST(I)
100         CONTINUE
C
C
            DO 200 I=1,NLINE
```

```fortran
        N     = NLEV(I)
        NTYPE= MOD(N,5)
        N     = N/5
        M     = MOD(N,20000)
        N     = N/20000
        J     = N/200
        KAF   = MOD(N/2,100)
        KCF   = J-KAF+MOD(N,2)
        JLO   = M/200
        KAI   = MOD(M/2,100)
        KCI   = JLO-KAI+MOD(M,2)
        RST   = ST(I)/SMAX
C
        IQR  = 1
        IF (J.EQ.JLO)  IQR=2
        IF (J.GT.JLO)  IQR=3
C
C
        WRITE(6,1000)  INTYPE(NTYPE),ITYP(IQR),J,KAF,KCF,JLO,
     1                 KAI,KCI,FRQ(I),ST(I),RST
200     CONTINUE
        RETURN
C
1000    FORMAT(5X,A1,3X,A1,3X,3I3,5X,3I3,F16.5,3X,1PE10.3,0PF8.4)
        END
        SUBROUTINE EIVEC(NS,A,B,ENERGY,T)
C       CALCULATION OF EIGENVECTOR
        IMPLICIT REAL*8(A-H,O-Z)
C       A   DIAGONAL ELMENTS OF TRIDIAGONAL MATRIX ( LARGEST
CTO SMALLER)
C       B  OFF DIAGONAL ELEMENTS
        DIMENSION A(50),B(50),T(50)
        IF (NS.GT.1)  GO TO 100
        T(1) = 1.0D0
        RETURN
100     WORK =DABS(A(1)-ENERGY)
        NU=1
        DO 10 I=2,NS
        WORKP=DABS(A(I)-ENERGY)
        IF(WORKP.GT.WORK) GO TO 10
        WORK=WORKP
        NU=I
10      CONTINUE
C       CALCULATE RATIO OF EIGENVECTOR
        IF(NU.GT.1) T(1)=-B(1)/(A(1)-ENERGY)
        IF(NU.LE.2) GO TO 18
        DO 17 J=2,NU-1
17      T(J)=-B(J)/(B(J-1)*T(J-1)+A(J)-ENERGY)
18      IF(NU.LT.NS) T(NS)=-B(NS-1)/(A(NS)-ENERGY)
        IF(NU.GE.NS-1) GO TO 20
        K=NS-1-NU
        DO 19 J=1,K
        JA=NS-J
```

```
19        T(JA)=-B(JA-1)/(B(JA)*T(JA+1)+A(JA)-ENERGY)
C         CALCULATE EIGEN-VECTOR
20        T(NU)=1.0
          T2=T(NU)**2
          IF(NU.EQ.1) GO TO 22
          DO 21 J=1,NU-1
          JA=NU-J
          T(JA)=T(JA+1)*T(JA)
21        T2=T2+T(JA)**2
22        IF(NU.EQ.NS) GO TO 24
          DO 23 J=NU+1,NS
          T(J)=T(J-1)*T(J)
23        T2=T2+T(J)**2
24        T2=1.0/DSQRT(T2)
          DO 25 J=1,NS
25        T(J)=T(J)*T2
          RETURN
          END
          SUBROUTINE DTSM(NS,Q,E)
C         DIAGONALIZATION OF TRIDIAGONAL MATRIX
          IMPLICIT REAL*8(A-H,O-Z)
C         Q   DIAGONAL  FROM THE LARGEST ELEMENT TO SMALLER
C         NS MUST BE LARGER THAN 1
          DIMENSION Q(50),E(50)
C         E   (QFF-DIAGONAL ELEMENT)**2
          PASS=0.1D-4
          E(NS)=0.0
          C=0.0
          NR=NS
C         SHIFT ORIGIN
5         RE2=DSQRT(E(1))
          CM=Q(1)-RE2
          DO 6 I=2,NR
          RE1=RE2
          RE2=DSQRT(E(I))
          CMP=Q(I)-RE1-RE2
          IF(CM.GT.CMP)CM=CMP
6         CONTINUE
          DO 7 I=1,NS
7         Q(I)=Q(I)-CM
          C=C+CM
          DO 8 I=2,NR
          E(I-1)=E(I-1)/Q(I-1)
8         Q(I)=Q(I)-E(I-1)
C         REPEAT ORTHOGONAL TRANSITION
          NROT=0
11        IF(NROT.GE.10) GO TO  102
          NROT=NROT+1
          Q(1)=Q(1)+E(1)
          DO 9 I=2,NR
          E(I-1)=Q(I)*E(I-1)/Q(I-1)
9         Q(I)=Q(I)-E(I-1)+E(I)
          IF(E(NR-1)-PASS) 103,11,11
```

```
102     DO 12 I=1,NR-1
        Q(I)=Q(I)+E(I)
12      E(I)=E(I)*Q(I+1)
        GO TO 5
103     NR=NR-1
        E(NR)=0.0
        IF(NR.GT.1) GO TO 102
        DO 10 I=1,NS
10      Q(I)=Q(I)+C
        RETURN
        END
C       CONSTRUCTION OF TRIDIAGONAL MATRIX
        SUBROUTINE MATRIX(ISYM,HDISYM,HOISYM,NH,KMAX,J)
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/CONST/A,B,C,DLJ,DLJK,DLK,DSJ,DSK,HLJ,HLJK,HLKJ,
     1    HLK,HSJ,HSJK,HSK
        DIMENSION HDISYM(50),HOISYM(50)
        KPAR=(ISYM-1)/2
        KMAX=(J+KPAR)/2*2-KPAR
        NH=(KMAX+2)/2
        IF(ISYM.EQ.2) NH=NH-1
        IF(NH.LE.0) NH=0
        IF(NH.EQ.0) RETURN
        JP=J*(J+1)
        BAVE = 0.5D0*(B+C)
        AP=A-BAVE
        BDIF =0.25D0*(B-C)
        FLJP =JP
        ADD=((HSJ*FLJP-DSJ+HSJK)*FLJP+BDIF-DSK+HSK)*FLJP
        BJJ=((HLJ*FLJP-DLJ)*FLJP+BAVE)*FLJP
        BJJ2=(HLJK*FLJP-DLJK)*FLJP+AP
        BJJ4=HLKJ*FLJP-DLK
        DO 10 I=1,NH
        K=KMAX+2-2*I
        FLKK=K*K
        HD=((HLK*FLKK+BJJ4)*FLKK+BJJ2)*FLKK+BJJ
        IF(K.NE.1) GO TO 10
        IF(ISYM.EQ.3) HD=HD+ADD
        IF(ISYM.EQ.4) HD=HD-ADD
10      HDISYM(I)=HD
        IF(NH.LE.1) RETURN
        BJJ=(HSJ*FLJP-DSJ+HSJK)*FLJP+BDIF-DSK+HSK
        BJJ2=HSJK*FLJP-DSK+6.0D0*HSK
        DO 20 I=1,NH-1
        K=KMAX+1-2*I
        FLKK=K*K
        HO=((HSK*FLKK+BJJ2)*FLKK+BJJ)*DSQRT(DBLE((JP-K*(K+1))
     1      *(JP-K*(K-1))))
        IF(K.EQ.1) HO=HO*DSQRT(2.0D0)
20      HOISYM(I)=HO
        RETURN
        END
```

```fortran
      SUBROUTINE SHAPE(NLINE)
C
C     THIS ROUTINE APPLIES A GAUSSIAN WITH HALFWIDTH = "WIDTH"
C     TO EACH BIN. AFTER THE LINESHAPE APPLICATION, IT WRITES
C     THE OUTPUT FILE CONTAINING THE LIMITS OF THE FREQUENCY
C     RANGE, NBINS, AND THE INTENSITY FOR EACH BIN.
C
      REAL INTEN,NORM
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
      COMMON /FREQ/ FMIN,FMAX
      COMMON /BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH
      COMMON/OTPUT/ACCESS2$
      COMMON/INTEN/TOTINT
      DIMENSION INTEN(200),SMOOTH(5000)
      CHARACTER*24 ACCESS2$
      OPEN (8,FILE=ACCESS2$,STATUS='NEW',ACCESS=
     1      'SEQUENTIAL')
      WRITE (8,2006) IDINT(FMIN),IDINT(FMAX)
      WRITE (6,2006) IDINT(FMIN),IDINT(FMAX)
      WRITE(8,2007) NBINS
2007  FORMAT(I5)
2006  FORMAT(I5,1H,,I5)
      NORM=SQRT(2.*ALOG(2.))/(WIDTH+1E-06)
      STEP=((FMAX-FMIN)/FLOAT(NBINS))*NORM
      X=STEP/2.
2009  FORMAT(1PE10.4)
      INTEN(1)=GAUSS(X)*2.
      SUM=INTEN(1)
      G=INTEN(1)/2.
      M=MIN1(200.,(5.0/SNGL(STEP))+1.)
      DO 20 J=2,M
      X=X+STEP
      INTEN(J)=-G
      G=GAUSS(X)
      INTEN(J)=G+INTEN(J)
20    SUM=SUM+2.*INTEN(J)
      BIG=0.0
      DO 50 I=1,NBINS
      SMOOTH(I)=BINST(I)*INTEN(1)
      DO 40 J=2,M
      K=I+J-1
      IF(K.LE.NBINS)SMOOTH(I)=SMOOTH(I)+BINST(K)*INTEN(J)
      K=I-J+1
40    IF(K.GE.1) SMOOTH(I)=SMOOTH(I)+BINST(K)*INTEN(J)
2002  FORMAT(I4,5X,F10.4,5X,F10.4)
2005  FORMAT(1PE9.3)
50    CONTINUE
C
C     TOTSMO IS THE SUM OF THE INTENSITES IN ALL BINS AFTER
C     THE GAUSSIAN LINESHAPE HAS BEEN APPLIED. BIG IS THE
C     MAXIMUM INTENSITY IN ANY OF THE BINS.
C
```

```fortran
      TOTSMO=0.0
      DO 49 I=1,NBINS
      TOTSMO=TOTSMO+SMOOTH(I)
      IF(SMOOTH(I).GE.BIG) BIG=SMOOTH(I)
C
C     THE INTENSITY IN EACH BIN SMOOTH(I) IS WRITTEN TO THE
C     OUTPUT FILE.
C
49    WRITE(8,2005) SMOOTH(I)
      WRITE (6,2011) TOTSMO
      WRITE(6,2012) BIG
2012  FORMAT(10X,'MAXIMUM INTENSITY = ',1PE10.4/)
2011  FORMAT(10X,'TOTAL BAND INTENSITY(GAUSSIAN SUM) = ',
     11PE10.4/)
      CLOSE (8)
      RETURN
      END
      REAL FUNCTION GAUSS(X)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(5)
      DATA B/1.3302744,-1.821256,1.7814779,-.35656378,.31938153/
      DATA P/.2316419/,Q/.39894228/
      T=1./(1.+P*X)
      PROD=0.0
      DO 10 I=1,5
10    PROD=T*(B(I)+PROD)
2010  FORMAT(3F10.6)
      GAUSS=0.5-Q*PROD*EXP(-(X**2/2.0))
      RETURN
      END
```

```fortran
      SUBROUTINE BINSORT(NLINE)
C
C     THIS ROUTINE SORTS THE STORED TRANSITIONS INTO BINS OF
C     EQUAL WIDTH AND SUMS THE INTENSITY IN EACH BIN.
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
      COMMON /FREQ/ FMIN,FMAX
      COMMON /BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH
C
C     THE BIN WIDTH DEL IS CALCULATED BY DIVIDING THE
C     FREQUENCY RANGE INTO NBINS EQUAL INCREMENTS.
C
      DEL=(FMAX-FMIN)/FLOAT(NBINS)
      K=1
      DO 100 I=1,NBINS
      BINST(I)=0.
      BINDEX(I)= FMIN+REAL(I*DEL)
      DO 200 J=K,NLINE
      IF(FRQ(J).LE.BINDEX(I)) THEN
        BINST(I) = BINST(I) + ST(J)
      IF(J.EQ.NLINE) GOTO 110
      ELSE
        K=J
        GO TO 150
      ENDIF
      IF(FRQ(J).GT.BINDEX(I)) K=J
200   CONTINUE
150   CONTINUE
100   CONTINUE
110   DO 50 L=I+1,NBINS
      BINST(L)=0.
50    CONTINUE
      RETURN
      END
```

```
ID[I3]
BU[E15.10]        DU[E15.10]        HU[E15.10]
BUQ[E15.10]       DUQ[E15.10]       HUQ[E15.10]
BL[E15.10]        DL[E15.10]        HL[E15.10]
JMIN[I4]          JMAX[I4]          FMIN[F10.4]       FMAX[F10.4]
FNU1[F16.8]       FNU2[F16.8]       FNU3[F16.8]
FNUZ[F16.8]       FLOW[F16.8]       FHIGH[F16.8]
SV[F16.8]         TT[F16.8]
NBINS[I5]         WIDTH[F10.6]
```

```
ID = identification code
BU,DU,HU = upper state constants
BUQ,DUQ,HUQ = upper state constants for other doublet level
BL,DL,HL = lower state constants
JMIN,JMAX = minimum and maximum values of J
FMIN,FMAX = minimum and maximum values of frequency
FNU1,FNU2,FNU3 = fundamental frequencies
FNUZ = band center
FLOW = lower state vibrational frequency
FHIGH = upper state vibrational frequency
SV = band strength
TT = temperature
NBINS = number of bins
WIDTH = Gaussian halfwidth
```

SAMPLE INPUT FILE CO2NU3

```
11
0.38714069        1.32873E-7        0.077E-13
0.00              0.00              0.00
0.39021817        1.33204E-7        0.055E-13
  0   20   2000.     2500.
1388.1847         667.3801          2349.1433
2349.1433         0000.             2349.1433
955900.           296.
5000   2.0
```

57

OUTPUT FROM PROGRAM CO2ABS

5/28/1987
13: 6

INPUT FILE = CO2NU3

OUTPUT FILE = CO2ANU3

ID = 11
UPPER STATE CONSTANTS
B =   0.38714069   D = 1.3287E-07   H = 7.7000E-15

UPPER STATE CONSTANTS(OTHER DOUBLET LEVEL)
B =   0.00000000   D = 0.0000E-01   H = 0.0000E-01
                .
LOWER STATE CONSTANTS
B =   0.39021817   D = 1.3320E-07   H = 5.5000E-15

J RANGE   0 TO   20
FREQUENCY RANGE   2000.0000 TO   2500.0000

BAND ORIGIN   2349.1433 CM-1
NU1   1388.1847 CM-1
NU2   667.3801 CM-1
NU3   2349.1433 CM-1

LOWER STATE VIBRATIONAL ENERGY =   0.0000 CM-1

UPPER VIBRATIONAL STATE ENERGY =   2349.1433 CM-1

BAND STRENGTH   955900.00000000
TEMPERATURE   296.0000
NBINS   5000
WIDTH   2.000000

P	20	2332.3694	1.128E+04	8.776261
P	18	2334.1569	1.178E+04	9.164751
P	16	2335.9199	1.197E+04	9.309935
P	14	2337.6586	1.179E+04	9.169424
P	12	2339.3728	1.120E+04	8.713461

P	10	2341.0625	1.019E+04	7.928887
P	8	2342.7277	8.770E+03	6.821999
P	6	2344.3685	6.968E+03	5.419867
P	4	2345.9847	4.846E+03	3.769805
P	2	2347.5763	2.490E+03	1.936939
R	0	2349.9176	1.261E+03	0.980531
R	2	2351.4477	3.741E+03	2.910200
R	4	2352.9531	6.076E+03	4.726255
R	6	2354.4338	8.164E+03	6.350329
R	8	2355.8899	9.922E+03	7.717874
R	10	2357.3212	1.129E+04	8.782356
R	12	2358.7277	1.224E+04	9.517692
R	14	2360.1095	1.275E+04	9.918749
R	16	2361.4664	1.286E+04	10.000000
R	18	2362.7985	1.259E+04	9.792624

2000, 2500

TOTAL BAND INTENSITY(GAUSSIAN SUM) = 1.8218E+05

MAXIMUM INTENSITY = 8.9935E+02

```fortran
C
C       PROGRAM CO2ABS.FOR
C
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION EL(500),EU(500),EROTP(500),EROTQ(500),
     1       EROTR(500),EP(500),EQ(500),ER(500),SP(500),
     1       SQ(500),SR(500),EUQ(500)
        COMMON/TBL/FRQ(1000),ST(1000),NLEV(1000)
        COMMON/FREQ/FMIN,FMAX
        COMMON/BINS/BINST(5000),BINDEX(5000),NBINS,WIDTH
        COMMON/OTPUT/ACCESS2$
        CHARACTER*8 FILENM1$,FILENM2$
        CHARACTER*24 ACCESS1$,ACCESS2$
        INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
        CALL GETTIM(IHOUR,IMINUTE)
        CALL GETDAT(IYEAR,IMONTH,IDAY)
        WRITE(6,*) ' ENTER INPUT FILENAME?'
        READ 19,FILENM1$
19      FORMAT(A8)
        WRITE(6,*) ' ENTER OUTPUT FILENAME?'
        READ 19, FILENM2$
        ACCESS1$='C:\ASYMRTR\'//FILENM1$//'.DAT'
        ACCESS2$='A:'//FILENM2$//'.DAT'
        OPEN(2,FILE=ACCESS1$,ACCESS='SEQUENTIAL')
        READ(2,23) ID
23      FORMAT(I3)
        READ(2,29) BU,DU,HU
29      FORMAT(3E15.10)
        READ(2,29) BUQ,DUQ,HUQ
        READ(2,29) BL,DL,HL
        READ(2,39) JMIN,JMAX,FMIN,FMAX
39      FORMAT(2I4,2F10.4)
        READ(2,29) FNU1,FNU2,FNU3
        READ(2,49) FNUZ,FLOW,FHIGH
49      FORMAT(3F16.8)
        READ(2,59) SV,TT
59      FORMAT(2F16.8)
        READ(2,69) NBINS,WIDTH
69      FORMAT(I5,F10.6)
        CLOSE(2)
        WRITE(6,1019)
1019    FORMAT(' OUTPUT FROM PROGRAM CO2ABS'//)
        WRITE(6,1025) IMONTH,IDAY,IYEAR
        WRITE(6,1026) IHOUR,IMINUTE
1025    FORMAT(1X,I2,'/',I2,'/',I4)
1026    FORMAT(1X,I2,':',I2/)
        WRITE(6,1029) FILENM1$
1029    FORMAT(' INPUT FILE = ',A8/)
        WRITE(6,1039) FILENM2$
1039    FORMAT(' OUTPUT FILE = ',A8/)
        WRITE(6,1024) ID
1024    FORMAT( ' ID = ',I3)
```

```
          WRITE(6,1049) BU,DU,HU
1049    FORMAT(' UPPER STATE CONSTANTS'/
     1          ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/)
          WRITE(6,1054) BUQ,DUQ,HUQ
1054    FORMAT(' UPPER STATE CONSTANTS(OTHER DOUBLET LEVEL) '/
     1          ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/)
          WRITE(6,1059) BL,DL,HL
1059    FORMAT(' LOWER STATE CONSTANTS'/
     1          ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/)
          WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
1069    FORMAT(//' J RANGE ',I4,' TO ',I4/
     1          ' FREQUENCY RANGE ',F10.4,' TO ',F10.4/)
          WRITE(6,1079) FNUZ,FNU1,FNU2,FNU3
1079    FORMAT(' BAND ORIGIN  ',F10.4,' CM-1'/
     1          ' NU1             ',F10.4,' CM-1'/
     2          ' NU2             ',F10.4,' CM-1'/
     3          ' NU3             ',F10.4,' CM-1'/)
          WRITE(6,1084) FLOW
1084    FORMAT(' LOWER STATE VIBRATIONAL ENERGY = ',F10.4,
     1' CM-1'/)
          WRITE(6,1086) FHIGH
1086    FORMAT(' UPPER VIBRATIONAL STATE ENERGY = ',F10.4,
     1' CM-1'/)
          WRITE(6,1089) SV,TT,NBINS,WIDTH
1089    FORMAT(' BAND STRENGTH ',F16.8/
     1          ' TEMPERATURE   ',F10.4/
     2          ' NBINS         ',I5/
     3 ' WIDTH            ',F10.6///)
          C2=1.438786
          NLINE=0
          DO 2000 I=JMIN,JMAX
          EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)*
     1((I+1)**3)
2000    CONTINUE
          DO 2500 I=JMIN,JMAX
          EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)*
     1((I=1)**3)
2500    CONTINUE
          DO 2600 I=JMIN,JMAX
          EUQ(I)=BUQ*I*(I+1)-DUQ*(I**2)*((I+1)**2)+
     1        HUQ*(I**3)*((I+1)**3)
2600    CONTINUE
          DO 3000 I=JMIN+2,JMAX,2
          EROTP(I)=EU(I-1)-EL(I)
3000    CONTINUE
          DO 3500 I=JMIN,JMAX-2,2
          EROTR(I)=EU(I+1)-EL(I)
3500    CONTINUE
          VIBPFT0=1./((1.-DEXP(-C2*FNU1/296.))*((1.-DEXP
     1          (-C2*FNU2/TT))**2)*(1.-DEXP(-C2*FNU3/296.)))
          VIBLZMT0=DEXP(-C2*FLOW/296.)
          ROTPFT0=296./BL
          VIBLZM=DEXP(-C2*FLOW/TT)
```

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```fortran
      ROTPF=TT/BL
      VIBPF=1./((1.-DEXP(-C2*FNU1/TT))*((1.-DEXP
     1        (-C2*FNU2/TT))**2)*(1.-DEXP(-C2*FNU3/TT)))
      S=(VIBLZM*SV*VIBPFT0)/(VIBLZMT0*VIBPF*ROTPF)
      IF(ID.LT.20) GO TO 3900
      DO 3600 I=JMIN+2,JMAX-2,2
      EROTQ(I)=EUQ(I)-EL(I)
3600  CONTINUE
      DO 3700 I=JMIN+2,JMAX-2,2
      FREQ=EROTQ(I) + FNUZ
      ROTBLZM=DEXP((-C2*EL(I)/TT))
      STIMEM = (1.-DEXP((-C2*FREQ)/TT))
      IF(ID.EQ.22) THEN
      HLFAC=(2.*REAL(I)+1.)/4.
      ELSE
      HLFAC=(2.*REAL(I)+1.)/((REAL(I))*(REAL(I)+1.))
      ENDIF
      SQ(I)=S*FREQ*HLFAC*STIMEM*ROTBLZM/FNUZ
      STRE=SQ(I)
      NTYPE=2000+I
      IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
      CALL STORE(NLINE,FREQ,STRE,NTYPE)
      ENDIF
3700  CONTINUE
3900  SMAX=0.000001
      DO 4000 I=JMIN+2,JMAX,2
      FREQ=EROTP(I)+FNUZ
      ROTBLZM=DEXP((-C2*EL(I))/TT)
      STIMEM=(1.-DEXP((-C2*FREQ)/TT).)
      IF(ID.EQ.11) THEN
      HLFAC=REAL(I)
      ELSEIF(ID.EQ.22) THEN
      HLFAC=REAL(I)*(REAL(I)-1)/(4.*REAL(I))
      ELSE
      HLFAC=(REAL(I)+1.)*(REAL(I)-1.)/REAL(I)
      ENDIF
      SP(I)=S*FREQ*HLFAC*STIMEM*ROTBLZM/FNUZ
      STRE=SP(I)
      NTYPE=1000+I
      IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
      CALL STORE(NLINE,FREQ,STRE,NTYPE)
      ENDIF
4000  CONTINUE
      DO 5000 I=JMIN,JMAX-2,2
      FREQ=EROTR(I)+FNUZ
      ROTBLZM=DEXP((-C2*EL(I)/TT))
      STIMEM=(1.-DEXP((-C2*FREQ)/TT))
      IF(ID.EQ.11) THEN
      HLFAC=REAL(I)+1.
      ELSEIF(ID.EQ.22) THEN
      HLFAC=(REAL(I)+2.)/4.
      ELSE
      HLFAC=(REAL(I)+2.)*REAL(I)/(REAL(I)+1.)
```

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```fortran
      ENDIF
      SR(I)=S*FREQ*HLFAC*STIMEM*ROTBLZM/FNUZ
      STRE=SR(I)
      NTYPE=3000+I
      IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
      CALL STORE(NLINE,FREQ,STRE,NTYPE)
      ENDIF
5000  CONTINUE
      CALL SORT(NLINE)
C     CALL PRINT(NLINE)
      CALL BINSORT(NLINE)
      CALL SHAPE(NLINE)
      STOP
      END
```

```
C       PROGRAM CO2EMS.FOR
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION EL(500),EU(500),EROTP(500),EROTQ(500),
     1        EROTR(500),EP(500),EQ(500),ER(500),SP(500),
     2        SQ(500),SR(500),EUQ(500)
        COMMON/TBL/FRQ(1000),ST(1000),NLEV(1000)
        COMMON/FREQ/FMIN,FMAX
        COMMON/BINS/BINST(5000),BINDEX(5000),NBINS,WIDTH
        COMMON/OTPUT/ACCESS2$
        CHARACTER*8 FILENM1$,FILENM2$
        CHARACTER*24 ACCESS1$,ACCESS2$
        INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
        CALL GETTIM(IHOUR,IMINUTE)
        CALL GETDAT(IYEAR,IMONTH,IDAY)
        WRITE(6,*) ' ENTER INPUT FILENAME?'
        READ 19,FILENM1$
19      FORMAT(A8)
        WRITE(6,*) ' ENTER OUTPUT FILENAME?'
        READ 19, FILENM2$
        ACCESS1$='C:\ASYMRTR\'//FILENM1$//'.DAT'
        ACCESS2$='A:'//FILENM2$//'.DAT'
        OPEN(2,FILE=ACCESS1$,ACCESS='SEQUENTIAL')
        READ(2,23) ID
23      FORMAT(I3)
        READ(2,29) BU,DU,HU
29      FORMAT(3E15.10)
        READ(2,29) BUQ,DUQ,HUQ
        READ(2,29) BL,DL,HL
        READ(2,39) JMIN,JMAX,FMIN,FMAX
39      FORMAT(2I4,2F10.4)
        READ(2,29) FNU1,FNU2,FNU3
        READ(2,49) FNUZ,FLOW,FHIGH
49      FORMAT(3F16.8)
        READ(2,59) SV,TT
59      FORMAT(2F16.8)
        READ(2,69) NBINS,WIDTH
69      FORMAT(I5,F10.6)
        CLOSE(2)
        WRITE(6,1019)
1019    FORMAT(' OUTPUT FROM PROGRAM CO2EMS'//)
        WRITE(6,1025) IMONTH,IDAY,IYEAR
        WRITE(6,1026) IHOUR,IMINUTE
1025    FORMAT(1X,I2,'/',I2,'/',I4)
1026    FORMAT(1X,I2,':',I2/)
        WRITE(6,1029) FILENM1$
1029    FORMAT(' INPUT FILE = ',A8/)
        WRITE(6,1039) FILENM2$
1039    FORMAT(' OUTPUT FILE = ',A8/)
        WRITE(6,1024) ID
1024    FORMAT( ' ID = ',I3)
        WRITE(6,1049) BU,DU,HU
1049    FORMAT(' UPPER STATE CONSTANTS'/
     1        ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4)
```

```
      WRITE(6,1054) BUQ,DUQ,HUQ
1054  FORMAT(' UPPER STATE CONSTANTS(OTHER DOUBLET LEVEL) '/
     1       ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/)
      WRITE(6,1059) BL,DL,HL
1059  FORMAT(' LOWER STATE CONSTANTS'/
     1       ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/)
      WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
1069  FORMAT(//' J RANGE ',I4,' TO ',I4/
     1       ' FREQUENCY RANGE ',F10.4,' TO ',F10.4/)
      WRITE(6,1079) FNUZ,FNU1,FNU2,FNU3
1079  FORMAT(' BAND ORIGIN  ',F10.4,' CM-1'/
     1       ' NU1             ',F10.4,' CM-1'/
     2       ' NU2             ',F10.4,' CM-1'/
     3       ' NU3             ',F10.4,' CM-1'/)
      WRITE(6,1084) FLOW
1084  FORMAT(' LOWER VIBRATIONAL STATE ENERGY = ',F10.4,
     1' CM-1'/)
      WRITE(6,1086) FHIGH
1086  FORMAT(' UPPER VIBRATIONAL STATE ENERGY = ',F10.4,
     1' CM-1'/)
      WRITE(6,1089) SV,TT,NBINS,WIDTH
1089  FORMAT(' BAND STRENGTH ',F16.8/
     1       ' TEMPERATURE    ',F10.4/
     2       ' NBINS          ',I5/
     3 ' WIDTH             ',F10.6///)
      C2=1.438786
      NLINE=0
      DO 2000 I=JMIN,JMAX
      EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)*
     1((I+1)**3)
2000  CONTINUE
      DO 2500 I=JMIN,JMAX
      EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)*
     1((I+1)**3)
2500  CONTINUE
      DO 2600 I=JMIN,JMAX
      EUQ(I)=BUQ*I*(I+1)-DUQ*(I**2)*((I+1)**2)+
     1       HUQ*(I**3)*((I+1)**3)
2600  CONTINUE
      DO 3000 I=JMIN+2,JMAX,2
      EROTP(I)=EU(I-1)-EL(I)
3000  CONTINUE
      DO 3500 I=JMIN,JMAX-2,2
      EROTR(I)=EU(I+1)-EL(I)
3500  CONTINUE
      VIBPFT0=1./((1.-DEXP(-C2*FNU1/296.))*((1.-DEXP
     1 (-C2*FNU2/296.))**2)*(1.-DEXP(-C2*FNU3/296.)))
      VIBLZMT0=DEXP(-C2*FLOW/296.)
      ROTPFT0=296./BL
      VIBLZM=DEXP(-C2*FHIGH/TT)
      ROTPF=TT/BL
      VIBPF=1./((1.-DEXP(-C2*FNU1/TT))*((1.-DEXP
     1       (-C2*FNU2/TT))**2)*(1.-DEXP(-C2*FNU3/TT)))
```

```fortran
          S=(VIBLZM*SV*VIBPFT0)/(VIBLZMT0*VIBPF*ROTPF)
          IF(ID.LT.20) GO TO 3900
          DO 3600 I=JMIN+2,JMAX-2,2
          EROTQ(I)=EUQ(I)-EL(I)
3600      CONTINUE
          DO 3700 I=JMIN+2,JMAX-2,2
          FREQ=EROTQ(I) + FNUZ
          ROTBLZM=DEXP((-C2*EL(I)/TT))
C         STIMEM = (1.-DEXP((-C2*FREQ)/TT))
          IF(ID.EQ.22) THEN
          HLFAC=(2.*REAL(I)+1.)/4.
          ELSE
          HLFAC=(2.*REAL(I)+1.)/((REAL(I))*(REAL(I)+1.))
          ENDIF
          SQ(I)=S*FREQ**4*HLFAC*ROTBLZM/FNUZ
          STRE=SQ(I)
          NTYPE=2000+I
          CALL STORE(NLINE,FREQ,STRE,NTYPE)
3700      CONTINUE
3900      SMAX=0.000001
          DO 4000 I=JMIN+2,JMAX,2
          FREQ=EROTP(I)+FNUZ
          ROTBLZM=DEXP((-C2*EL(I))/TT)
C         STIMEM=(1.-DEXP((-C2*FREQ)/TT))
          IF(ID.EQ.11) THEN
          HLFAC=REAL(I)
          ELSEIF(ID.EQ.22) THEN
          HLFAC=REAL(I)*(REAL(I)-1)/(4.*REAL(I))
          ELSE
          HLFAC=(REAL(I)+1.)*(REAL(I)-1.)/REAL(I)
          ENDIF
          SP(I)=S*FREQ**4*HLFAC*ROTBLZM/FNUZ
          STRE=SP(I)
          NTYPE=1000+I
          CALL STORE(NLINE,FREQ,STRE,NTYPE)
4000      CONTINUE
          DO 5000 I=JMIN,JMAX-2,2
          FREQ=EROTR(I)+FNUZ
          ROTBLZM=DEXP((-C2*EL(I)/TT))
C         STIMEM=(1.-DEXP((-C2*FREQ)/TT))
          IF(ID.EQ.11) THEN
          HLFAC=REAL(I)+1.
          ELSEIF(ID.EQ.22) THEN
          HLFAC=(REAL(I)+2.)/4.
          ELSE
          HLFAC=(REAL(I)+2.)*REAL(I)/(REAL(I)+1.)
          ENDIF
          SR(I)=S*FREQ**4*HLFAC*ROTBLZM/FNUZ
          STRE=SR(I)
          NTYPE=3000+I
          CALL STORE(NLINE,FREQ,STRE,NTYPE)
5000      CONTINUE
          CALL SORT(NLINE)
```

```
CALL  PRINT(NLINE)
CALL  BINSORT(NLINE)
CALL  SHAPE(NLINE)
STOP
END
```

```
C        PROGRAM HCLEMS
         IMPLICIT REAL*8(A-H,O-Z)
         DIMENSION EL(1000),EU(1000),EROTP(1000),EROTR(1000),
     1        EP(1000),ER(1000),SP(1000),SR(1000)
         COMMON/TBL/FRQ(10000),ST(10000)
         COMMON/FREQ/FMIN,FMAX
         COMMON/BINS/BINST(5000),BINDEX(5000),NBINS,WIDTH
         COMMON/OTPUT/ACCESS2$
         COMMON/INTEN/TOTINT,STRENGTH
         CHARACTER*8 FILENM1$,FILENM2$
         CHARACTER*24 ACCESS1$,ACCESS2$
         WRITE(6,*) ' ENTER INPUT FILENAME?'
         READ 19,FILENM1$
19       FORMAT(A8)
         WRITE(6,*) ' ENTER OUTPUT FILENAME?'
         READ 19, FILENM2$
         ACCESS1$='C:\ASYMRTR\'//FILENM1$//'.DAT'
         ACCESS2$='A:'//FILENM2$//'.DAT'
         OPEN(2,FILE=ACCESS1$,ACCESS='SEQUENTIAL')
         READ(2,29) BU,DU,HU
29       FORMAT(3F16.10)
         READ(2,29) BL,DL,HL
         READ(2,39) JMIN,JMAX,FMIN,FMAX
39       FORMAT(2I4,2F10.4)
         READ(2,49) FNUZ
49       FORMAT(F16.8)
         READ(2,59) SV,TT
59       FORMAT(2F16.8)
         READ(2,69) NBINS,WIDTH
69       FORMAT(I5,F10.6)
         CLOSE(2)
         WRITE(6,1019)
1019     FORMAT(' OUTPUT FROM PROGRAM HCL'//)
         WRITE(6,1029) FILENM1$
1029     FORMAT(' INPUT FILE = ',A8/)
         WRITE(6,1039) FILENM2$
1039     FORMAT(' OUTPUT FILE = ',A8/)
         WRITE(6,1049) BU,DU,HU
1049     FORMAT(' UPPER STATE CONSTANTS'/
     1        ' B = ',F16.8,'D = ',F16.8,'H = ',F16.8/)
         WRITE(6,1059) BL,DL,HL
1059     FORMAT(' LOWER STATE CONSTANTS'/
     1        ' B = ',F16.8,'D = ',F16.8,'H = ',F16.8/)
         WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
1069     FORMAT(//' J RANGE ',I4,' TO ',I4/
     1        ' FREQUENCY RANGE ',F10.4,' TO ',F10.4/)
         WRITE(6,1079) FNUZ
1079     FORMAT(' BAND ORIGIN  ',F10.4,' CM-1'/)
         WRITE(6,1089) SV,TT,NBINS,WIDTH
1089     FORMAT(' BAND STRENGTH ',F16.8/
     1        ' TEMPERATURE   ',F10.4/
     2        ' NBINS         ',I5/
     3   ' WIDTH         ',F10.6///)
```

```
            C2=1.438786
            NLINE=0
            TOTINT=0.0
            DO 2000 I=JMIN,JMAX
            EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)*
          1((I+1)**3)
 1100       FORMAT(' J= ',I4,' ER= ',F10.4)
 2000       CONTINUE
            DO 2500 I=JMIN,JMAX
            EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)*
          1((I+1)**3)
 2500       CONTINUE
            DO 3000 I=JMIN+1,JMAX
            EROTP(I)=EU(I-1)-EL(I)
 3000       CONTINUE
            DO 3500 I=JMIN,JMAX
            EROTR(I)=EU(I+1)-EL(I)
 3500       CONTINUE
            VIBPFT0=1./(1.-DEXP(-C2*FNUZ/296.))
            VIBLZMT0=DEXP(-C2*FNUZ/296.)
            ROTPFT0=296./BL
            VIBLZM=DEXP(-C2*FNUZ/TT)
            ROTPF=TT/BL
            VIBPF=1./(1.-DEXP(-C2*FNUZ/TT))
            SMAX=0.0001
            DO 4000 I=JMIN+1,JMAX
            FREQ=EROTP(I)+FNUZ
            ROTBLZM=DEXP((-C2*EU(I))/TT)
            HLFAC=I
            MM=-I
            FF=1.+(-2.5599E-2)*MM+(3.203E-4)*MM**2
            STRENGTH=HLFAC*ROTBLZM/ROTPF
            SP(I)=FREQ**4*VIBLZM*VIBPFT0*FF*STRENGTH/
          :        (FNUZ*VIBPF)
            IF(SP(I).GT.SMAX) SMAX=SP(I)
            EP(I)=FREQ
            STRE=SP(I)
 1099       FORMAT(' P ',3X,I4,5X,F10.4,5X,1PE9.3,5X,F10.6)
            IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
            CALL STORE(NLINE,FREQ,STRE)
            ENDIF
 4000       CONTINUE
            DO 5000 I=JMIN,JMAX-1
            FREQ=EROTR(I)+FNUZ
            ROTBLZM=DEXP((-C2*EU(I)/TT))
            HLFAC=I+1.
            MM=I+1.
            FF=1.+(-2.5599E-2)*MM+(3.203E-4)*MM**2
            STRENGTH=HLFAC*ROTBLZM/ROTPF
            SR(I)=FREQ**4*VIBLZM*VIBPFT0*FF*STRENGTH/
          1        (FNUZ*VIBPF)
            IF(SR(I).GT.SMAX) SMAX=SR(I)
            ER(I)=FREQ
```

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```fortran
      STRE=SR(I)
      IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
      CALL STORE(NLINE,FREQ,STRE)
      ENDIF
 5000 CONTINUE
      DO 6000 I = JMAX,JMIN+1,-1
      SREL = SP(I)/SMAX
      WRITE(6,1099) I,EP(I),SP(I),SREL
 6000 CONTINUE
      DO 7000 I=JMIN,JMAX-1
      SREL=SR(I)/SMAX
      WRITE(6,1109) I,ER(I),SR(I),SREL
 1109 FORMAT(' R ',3X,I4,5X,F10.4,5X,1PE9.3,5X,F10.6)
 7000 CONTINUE
      WRITE(6,1119) TOTINT
 1119 FORMAT(' TOTINT =  ',F10.6)
      CALL SORT(NLINE)
      CALL BINSORT(NLINE)
      CALL SHAPE(NLINE)
      STOP
      END
```

Table 1 - Statistical Weight Factors for Isotopes of Water

Isotope	Value of $|\tau|$	Symmetry	Relative Weight
H_2O	odd	antisymmetric	3
	even	symmetric	1
D_2O	odd	antisymmetric	3
	even	symmetric	6
HDO	odd or even	no identical nuclei	1

Table 2 - Hönl-London Factors for CO_2

	$\Delta J = -1$ (P)	$\Delta J = 0$ (Q)	$\Delta J = +1$ (R)
$\Delta \ell = 0$			
$\Sigma - \Sigma$ bands	J	---	$J + 1$
$\Pi - \Pi$ bands	$\dfrac{(J+1)(J-1)}{J}$	$\dfrac{(2J+1)}{J(J+1)}$	$\dfrac{J(J+2)}{J+1}$
$\Delta \ell = +1$			
$\Pi - \Sigma$ bands	$\dfrac{J(J-1)}{4J}$	$\dfrac{2J+1}{4}$	$\dfrac{J+2}{4}$

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Table 3 - Constants for H_2O Calculations

Rotational Constants (in cm^{-1})

$v_1 v_2 v_3$	000[9]	100[10]	010[9]	001[10]	020[10]
A	27.88067	27.1221_7	31.1283_5	26.6480_5	35.5867_2
B	14.52168_9	14.3047_7	14.68756_9	14.43130_2	14.8415_4
C	9.27745_9	9.1045_7	9.12913_2	9.13816_7	8.9744_8
$\Delta_J \times 10^3$	1.2489_4	1.233_0	1.3953_7	1.3054_9	1.580_4
$\Delta_{JK} \times 10^3$	-5.765_5	-5.387_4	-7.605_3	-5.656_1	-10.48_8
$\Delta_K \times 10^2$	3.2519_9	3.023_0	5.755_{6+}	2.858_4	10.991_0
$\delta_J \times 10^4$	5.083_8	4.998_7	5.787_9	5.381_7	6.75_2
$\delta_K \times 10^3$	1.300_7	1.240_5	3.766_2	1.326_1	8.71_1

Vibrational Constants[8]

v'	v''	$\nu_0(cm^{-1})$	$S_v^0 \times 10^{20}$(cm molecule)	Band Type
100	000	3657.053	48.62	B
010	000	1594.778	1038.0	B
001	000	3755.930	692.5	A
020	000	3151.630	7.537	B

Table 4 - Constants for D_2O Calculation

Rotational Constants

$v_1 v_2 v_3$	000[11]	100[11]	010[12]	001[11]
$A(cm^{-1})$	15.3846	15.1286	16.633880_2	14.7916
$B(cm^{-1})$	7.2716	7.1696	7.338823_1	7.2266
$C(cm^{-1})$	4.8458	4.7698	4.789485_8	4.7908

Vibrational Constants

v'	v''	$\nu_0(cm^{-1})$[13]	$S_v^0 \times 10^{20}(cm/molecule)$[14]	Band Type
100	000	2672.0811	34.0	B
010	000	1178.374	564.	B
001	000	2787.7182	486.	A

Table 5 - Constants for HDO Calculation

Rotational Constants

$v_1 v_2 v_3$	000[15]	100[16]	010[17]	001[13]	020[16]
$A(cm^{-1})$	23.413842 .	23.09585_4	25.551	22.3226	28.25549_8
$B(cm^{-1})$	9.103323	8.92521_5	9.238	9.0850	9.36779_7
$C(cm^{-1})$	6.406295	6.304243_0	6.335	6.3293	6.240077_8

Vibrational Constants

v'	v''	$\nu_0(cm^{-1})$[15]	$S_v^0 \times 10^{20}$(cm/molecule)	Band Type
100	000	2723.680	215. [18]	A
100	000	2723.680	1.73 [18]	B
010	000	1403.421	406.2 [19]	A
010	000	1403.421	532.8 [19]	B
001	000	3707.47	350.3 [20]	A
001	000	3707.47	145.3 [20]	B
020	000	2782.012	24.2 [18]	A
020	000	2782.012	11.1 [18]	B

Table 6 - Constants for CO_2 Calculation

Rotational Constants[7]

v^*	$G_v(cm^{-1})$	$B(cm^{-1})$	$D \times 10^7(cm^{-1})$	$H \times 10^{13}(cm^{-1})$
00001	0.	0.39021817	1.33204	0.055
01101 e	667.3801	0.39063825	1.35133	
01101 f	667.3801	0.39125388	1.35900	
00011	2349.1433	0.38714069	1.32873	0.077
01111 e	3004.0122	0.38759172	1.34546	
01111 f	3004.0122	0.38818943	1.35522	
10012	3612.8417	0.38750237	1.57314	2.024
10011	3714.7828	0.38706251	1.14177	1.989

*For band notation, see[3], pp. 23-24

Vibrational Constants[7]

$\nu_0(cm^{-1})$	v'	v''	$S_v^0 \times 10^{20}(cm/molecule)$	Band Type
667.380	01101	00001	82580.	$\Pi_u - \Sigma_g^+$
2336.632	01111	01101	73700.	$\Pi_g - \Pi_u$
2349.143	00011	00001	955900.	$\Sigma_u^+ - \Sigma_g^+$
3612.842	10012	00001	10400.	$\Sigma_u^+ - \Sigma_g^+$
3714.783	10011	00001	15800.	$\Sigma_u^+ - \Sigma_g^+$

Table 7 – Constants for HCℓ Calculations

Rotational Constants[24]

	$B(cm^{-1})$	$D(cm^{-1})$
$H^{35}Cℓ(v=0)$	10.4400	0.000530
$H^{35}Cℓ(v=1)$	10.1381	0.000526
$D^{35}Cℓ(v=0)$	5.392149	0.0001397
$D^{35}Cℓ(v=1)$	5.278858	0.0001410

Vibrational Constants[24]

	$\nu_o(cm^{-1})$
$H^{35}Cℓ$	2885.82
$D^{35}Cℓ$	2091.079
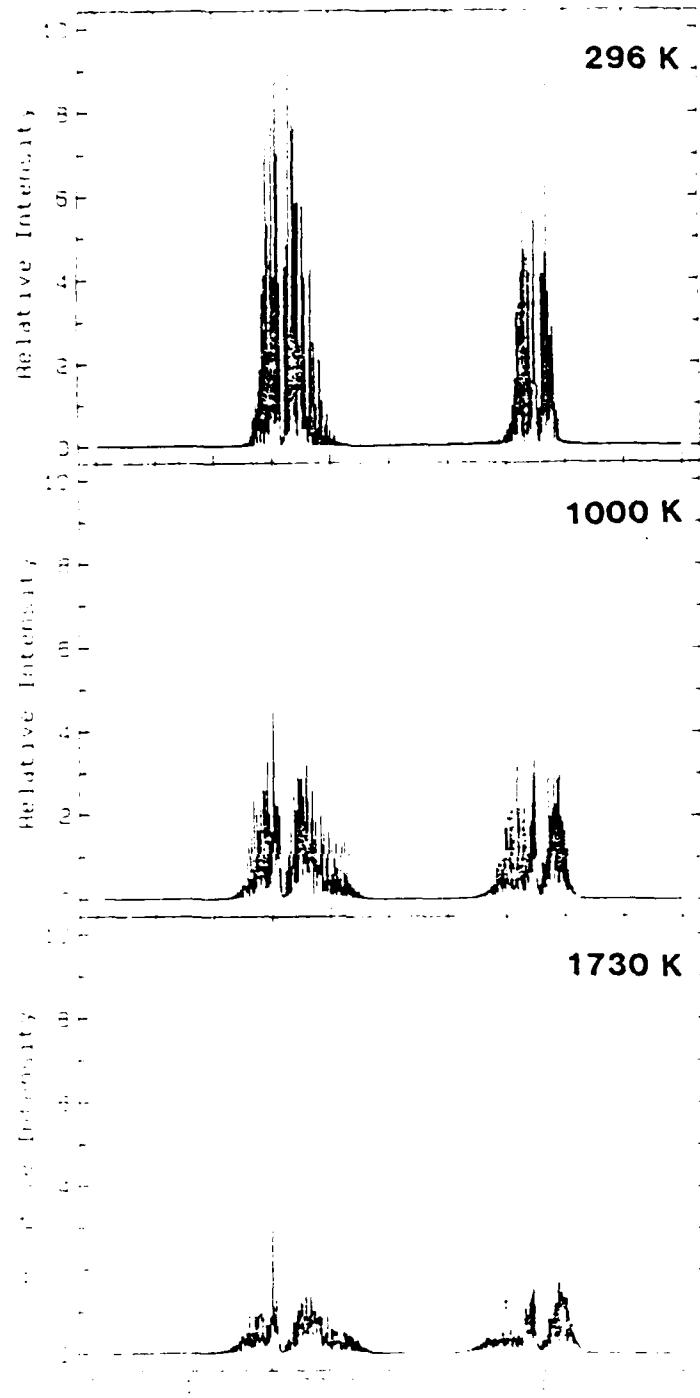
Fig. 1 - Simulated absorption spectra of H_2O at 296K, 1000K, and 1730K.

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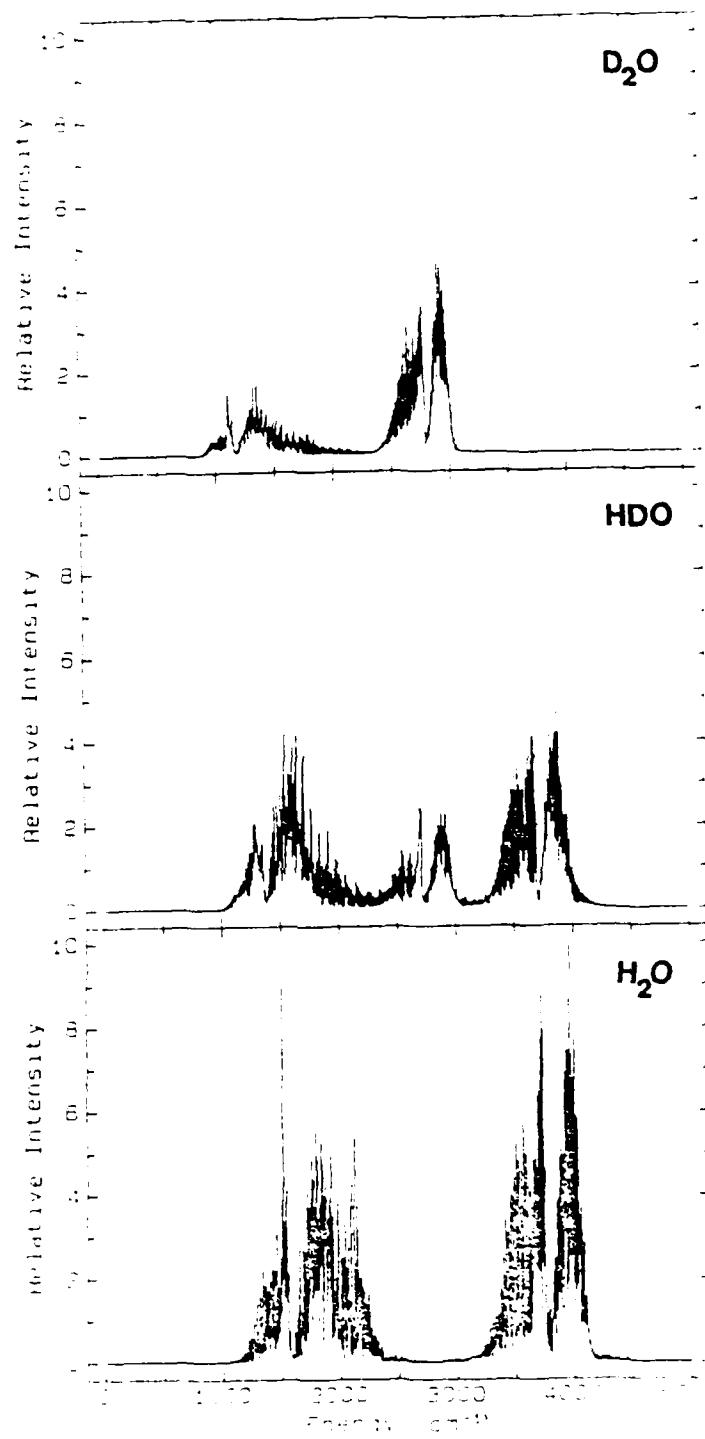
Fig. 2 - Simulated emission spectra of D_2O, HDO and H_2O at 1730K.
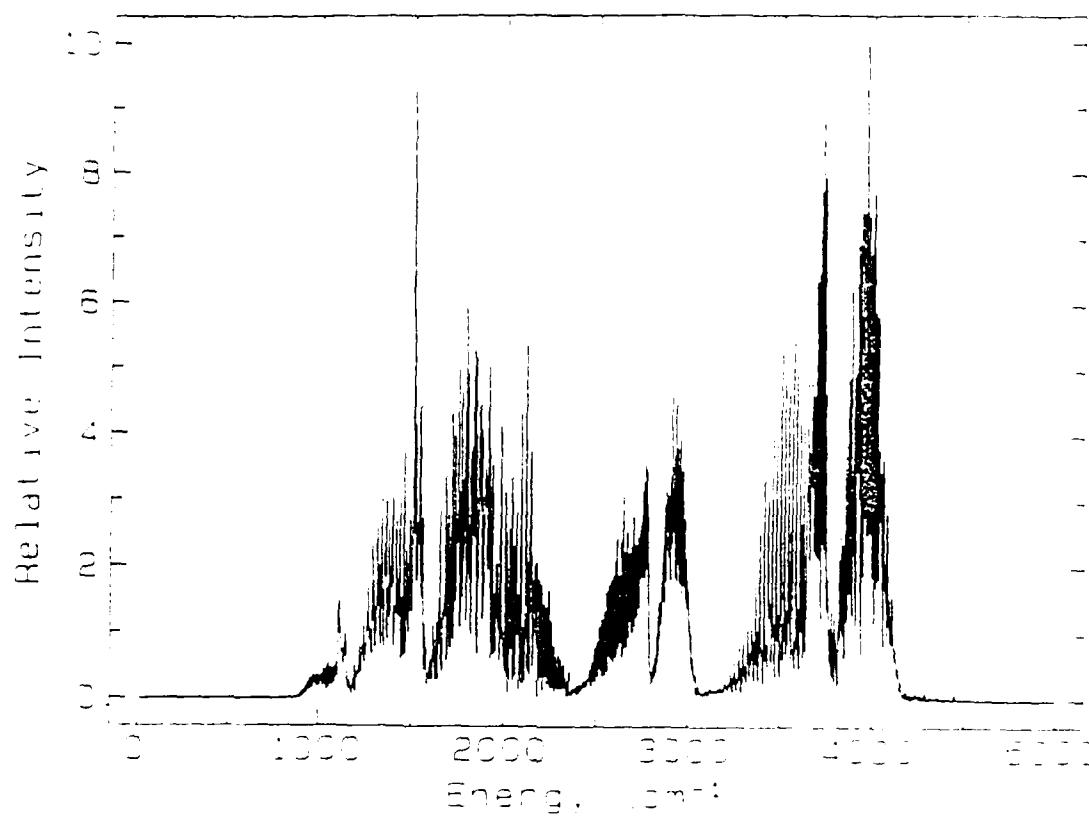
Fig. 3 - Simulated emission spectrum of an equimolar H_2O-D_2O mixture at 1730K.
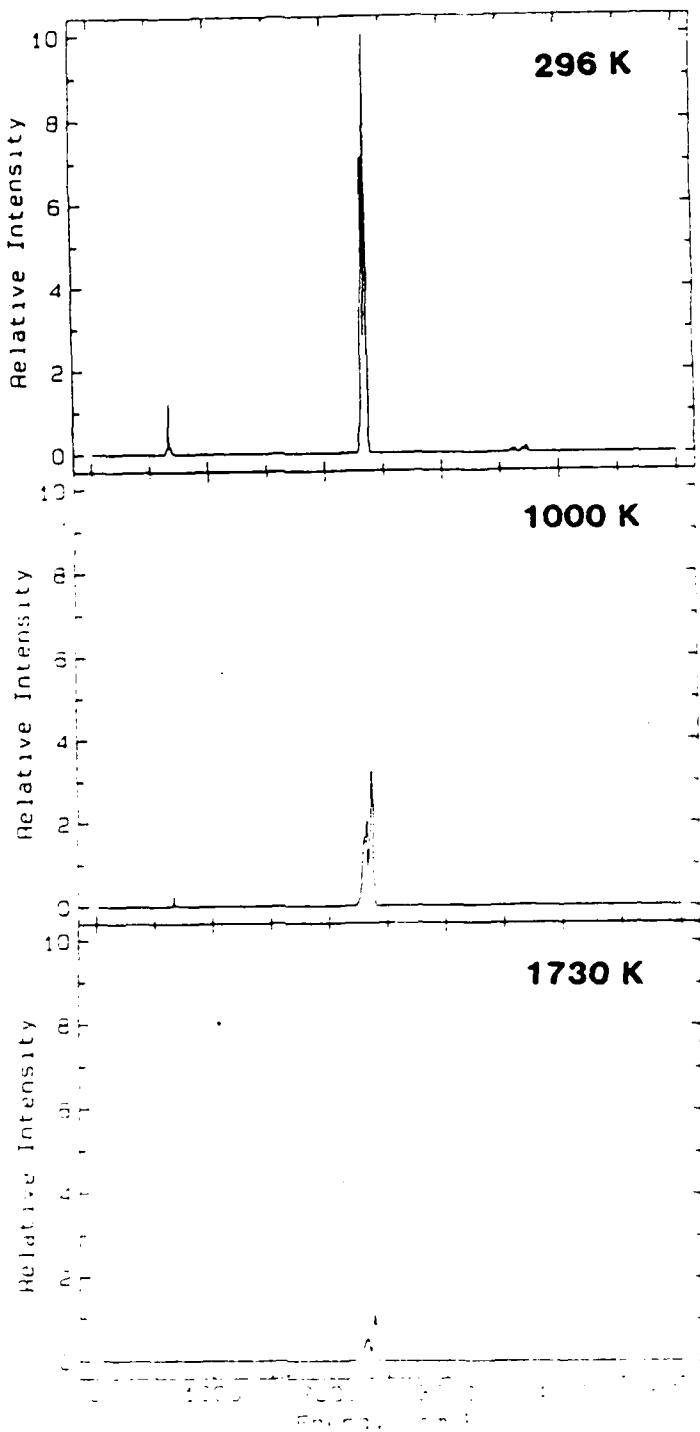
Fig. 4 - Simulated absorption spectra of CO_2 at 296K, 1000K, and 1730K.
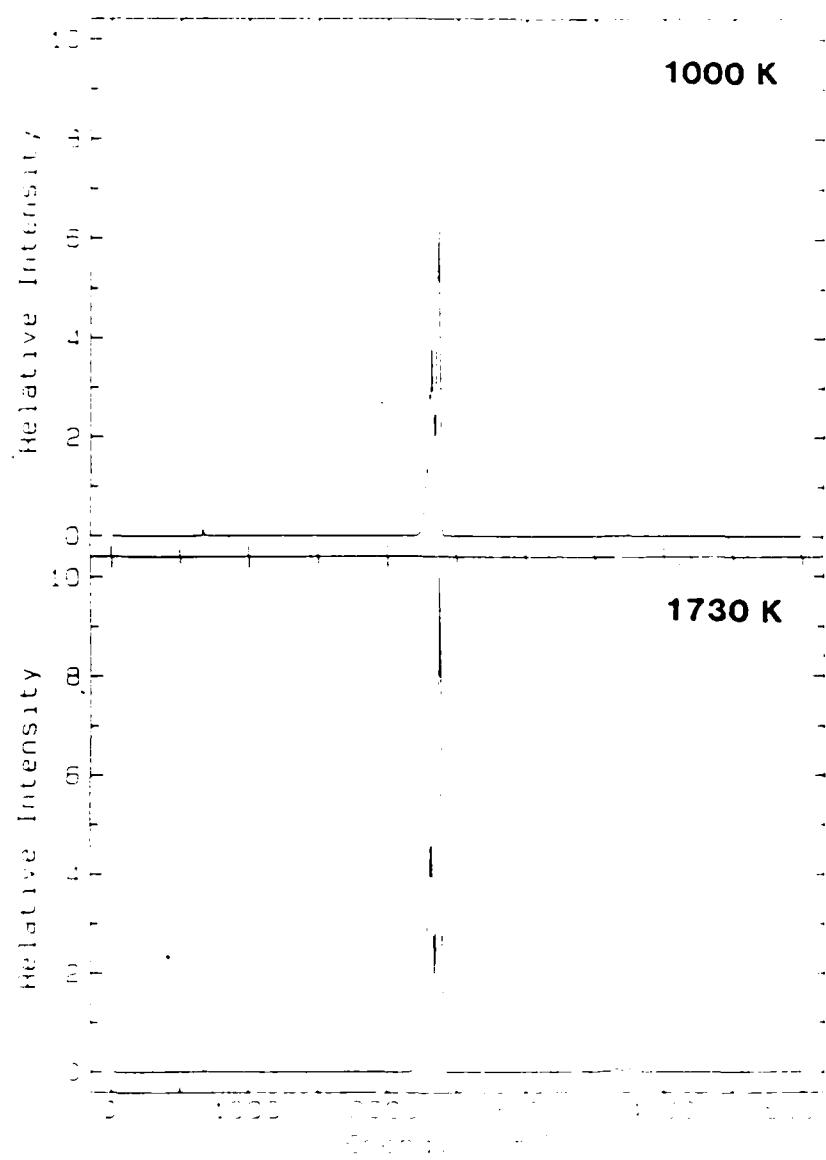
Fig. 5 - Simulated emission spectra of CO_2 at 1000K and 1730K.
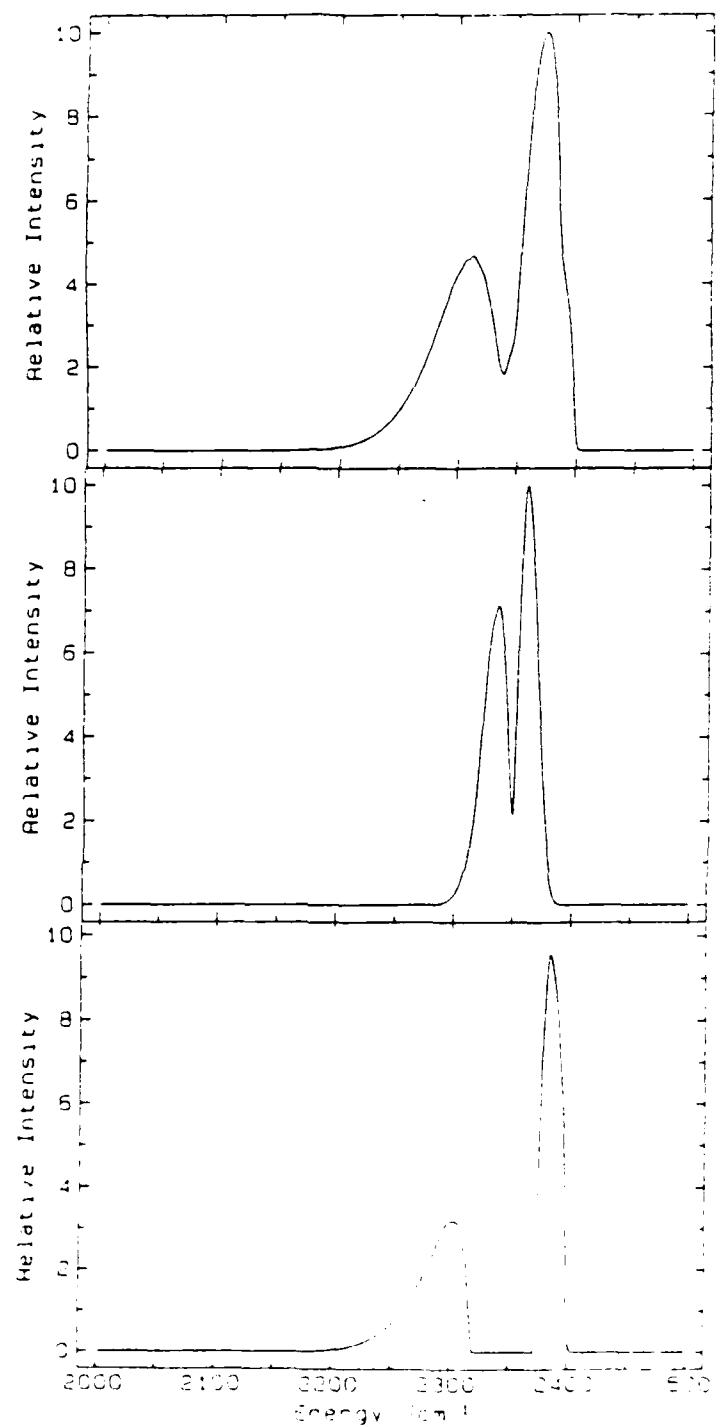
Fig. 6 – Simulation of hot CO_2 emission spectrum at 1730K, cold CO_2 absorption spectrum at 296K, and hot CO_2 emission viewed through absorbing cold CO_2.
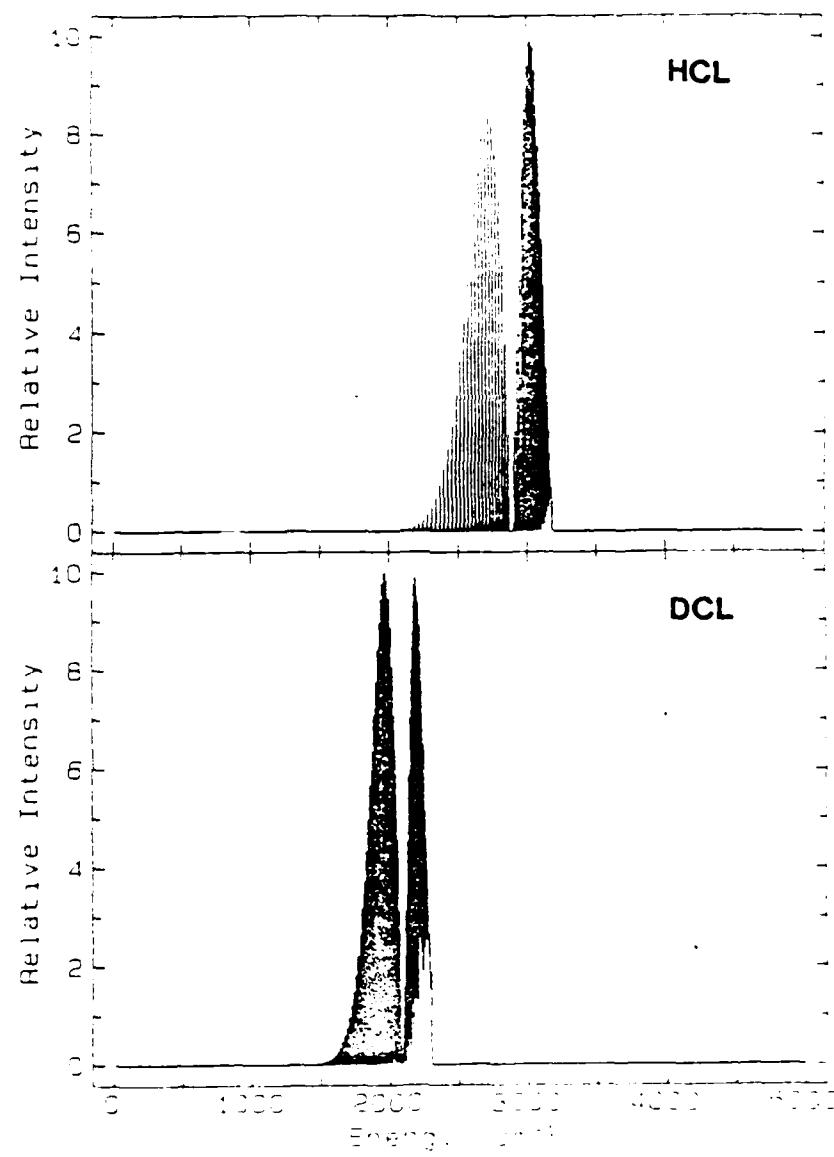
Fig. 7 - Simulated emission spectra of HCℓ and DCℓ at 1730K.

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